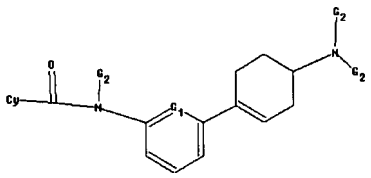
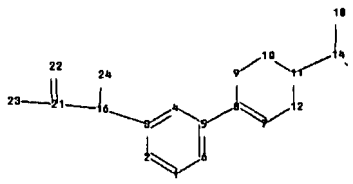
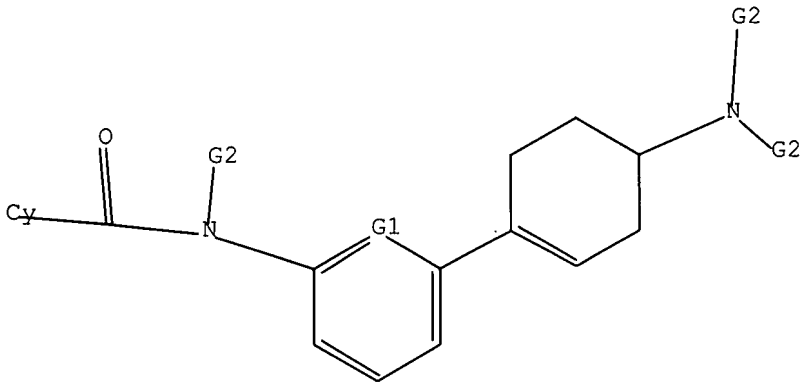
```
* * * * * * * * *   Welcome to STN International   * * * * * * * * * *
* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:30:04 ON 20 SEP 2007

=> file reg
=>Uploading C:\Program Files\Stnexp\Queries\Queries\10576762.str
```





```
chain nodes :
14  16  18  19  21  22  23  24
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12
chain bonds :
3-16  5-8  11-14  14-19  14-18  16-21  16-24  21-22  21-23
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
exact/norm bonds :
1-2  1-6  2-3  3-4  3-16  4-5  5-6  5-8  7-8  7-12  8-9  9-10  10-11  11-12  11-14
14-19  14-18  16-21  16-24  21-22  21-23
isolated ring systems :
containing 1 : 7 :


G1:C,N

G2:H,Ak

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  14:CLASS  16:CLASS  18:CLASS  19:CLASS  21:CLASS  22:CLASS
23:Atom  24:CLASS



L1      STRUCTURE UPLOADED

=> dis l1
L1 HAS NO ANSWERS
L1              STR
```



G1 C,N
G2 H,Ak

Structure attributes must be viewed using STN Express query preparation.

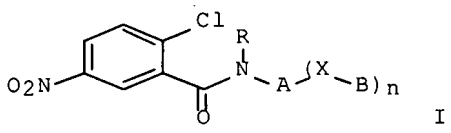
```
=> s l1 sam
L2             3 SEA SSS SAM L1

=> s l1 full
L3           127 SEA SSS FUL L1

=> file caplus

=> s l3
L4            32 L3

=> s l4 and pd< dec 2003
      23857158 PD< DEC 2003
                  (PD<20031200)
L5            22 L4 AND PD< DEC 2003

=> dis l5 1-22 bib abs hitstr

L5   ANSWER 1 OF 22  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2003:335065  CAPLUS  Full-text
DN   138:368620
TI   Preparation of 2-chloro-5-nitrobenzamides as lipid modulators for
     treatment of osteoporosis and diabetes
IN   Amemiya, Yoshiya; Wakabayashi, Kenji; Takaishi, Sachiko; Kitayama, Ken
PA   Sankyo Company, Limited, Japan
SO   PCT Int. Appl., 221 pp.
     CODEN: PIXXD2
DT   Patent
LA   Japanese
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    --------------------   --------
PI   WO 2003035602        A1    20030501    WO 2002-JP11068        20021024 <--
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
```

UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002338204	A1	20030506	AU 2002-338204	20021024	<--
JP 2003201271	A	20030718	JP 2002-310549	20021025	<--
PRAI JP 2001-327189	A	20011025			
WO 2002-JP11068	W	20021024			

OS MARPAT 138:368620

GI



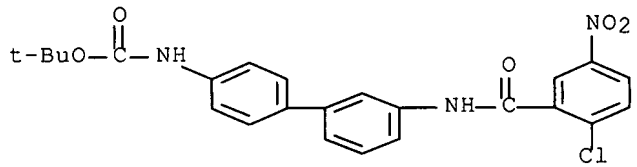
I

AB The title compds. I [wherein A = (un)substituted Ph, naphthyl, acenaphthenyl, Py, (iso)quinolyl, pyrimidyl, (benzo)furyl, pyranyl, chromanyl, (benzo)thienyl, pyrrolyl, (iso)indolyl, imidazolyl, pyrazolyl, pyridazinyl, pyrazinyl, (iso)oxazolyl, pyrrolidinyl, piperidyl, piperazyl, benzoxazolyl, benzoisooxazolyl, (iso)thiazolyl, benzothiazolyl, or biphenyl; B = (un)substituted aryl, cycloalkyl, or heterocyclyl; R = H or alkyl; X = a bond, O, S, CH2, CO, NH, SO2NH, NHSO2, CONH, NHCO, or OCH2; n = 0-1] and pharmaceutically acceptable salts thereof are prepared as lipid modulators for treatment of osteoporosis and diabetes. For example, 4-phenylaniline hydrochloride was reacted with 2-chloro-5-nitrobenzoyl chloride in pyridine to afford N-(4-phenylphenyl)-2-chloro-5- nitrobenzamide. The above N-(4-phenylphenyl)-2-chloro-5-nitrobenzamide showed IC50 of 1.9 nM against human PPAR γ. I are useful for the treatment of osteoporosis, and diabetes, etc.

IT 518991-67-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of chloro(nitro)benzamides as lipid modulators for treatment of osteoporosis and diabetes)

RN 518991-67-8 CAPLUS

CN Carbamic acid, [3'-[(2-chloro-5-nitrobenzoyl)amino][1,1'-biphenyl]-4-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

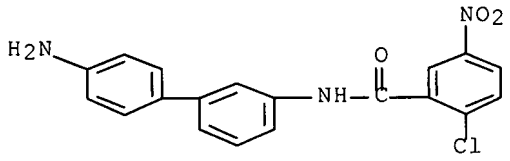


IT 518991-69-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of chloro(nitro)benzamides as lipid modulators

for treatment of osteoporosis and diabetes)

RN 518991-69-0 CAPLUS

CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)-2-chloro-5-nitro- (9CI) (CA INDEX NAME)



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:174344 CAPLUS Full-text

DN 138:221700

TI Preparation and uses of conjugated solid supports for boronic acids

IN Hall, Dennis G.

PA The Governors of The University of Alberta, Can.

SO U.S. Pat. Appl. Publ., 45 pp.
CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003044840	A1	20030306	US 2001-943465	20010831 <--
	US 6919382	B2	20050719		
	CA 2356455	A1	20020228	CA 2001-2356455	20010831 <--
PRAI	US 2000-229833P	P	20000831		
	US 2000-235386P	P	20000925		
	CA 2000-2317191	A	20000831		

OS CASREACT 138:221700

AB The invention provides novel solid supports comprising dihydroxyalkyl aminoalkyl and dihydroxyalkylaminobenzyl groups [e.g., N,N-diethanolaminomethyl polystyrene, (I)], and methods for making and using them. The supports are particularly useful for immobilizing and derivatizing functionalized boronic acids for use in solid phase synthesis, such as those used in combinatorial chemistries. For example, when I is coupled with p-MeC6H4B(OH)2 the corresponding resin bound arylboronic acid is formed nearly quant. The compns. and methods of the invention are also useful as scavenger solid supports, e.g., in solution-phase parallel synthesis of small mol. libraries, and for use in resin-to-resin transfer reactions via phase transfer of solid supported boronic acids under both aqueous and anhydrous conditions. The methods of the invention provide convergent solid-phase synthesis of sym. or unsym. functionalized compds., such as biphenyl compds. Also provided are synthesizer devices, e.g., semiautomated parallel synthesizers.

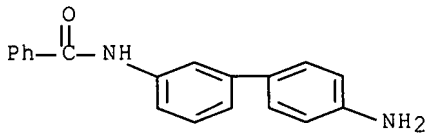
IT 268748-37-4P 268748-39-6P 268748-41-0P
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(preparation and uses of conjugated solid supports for boronic acids)

RN 268748-37-4 CAPLUS

CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

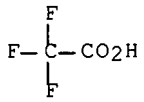
CM 1

CRN 268748-30-7
CMF C19 H16 N2 O



CM 2

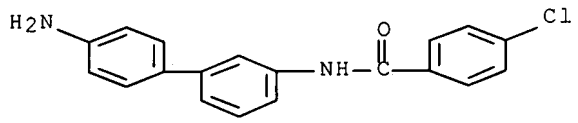
CRN 76-05-1
CMF C2 H F3 O2



RN 268748-39-6 CAPLUS
CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)-4-chloro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

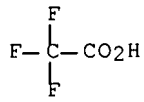
CM 1

CRN 268748-38-5
CMF C19 H15 Cl N2 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

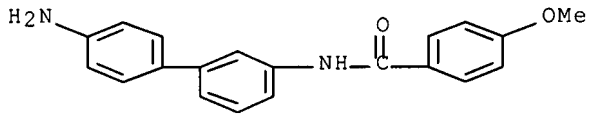


RN 268748-41-0 CAPLUS

CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)-4-methoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

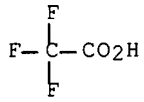
CM 1

CRN 268748-40-9
CMF C20 H18 N2 O2

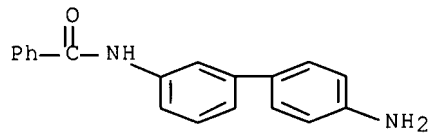


CM 2

CRN 76-05-1
CMF C2 H F3 O2



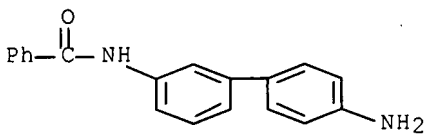
IT 268748-30-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and uses of conjugated solid supports for boronic acids)
RN 268748-30-7 CAPLUS
CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)- (9CI) (CA INDEX NAME)



RE.CNT 122 THERE ARE 122 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:870423 CAPLUS Full-text
DN 136:167426
TI Universal Solid-Phase Approach for the Immobilization, Derivatization, and Resin-to-Resin Transfer Reactions of Boronic Acids
AU Gravel, Michel; Thompson, Kim A.; Zak, Mark; Berube, Christian; Hall, Dennis G.
CS Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.
SO Journal of Organic Chemistry (2002), 67(1), 3-15
CODEN: JOCEAH; ISSN: 0022-3263

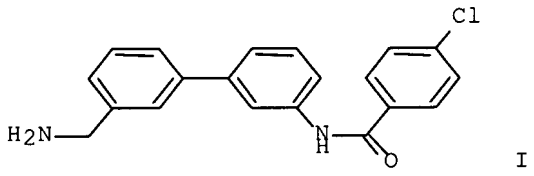
PB American Chemical Society
DT Journal
LA English
OS CASREACT 136:167426
AB Boronic acid-containing mols. are employed in a broad range of biol., medicinal, and synthetic applications. These compds., however, tend to be difficult to handle by solution-phase methods. Herein, this problem is addressed with the development of the first general solid-phase approach for the derivatization of functionalized boronic acids. This approach is based on the use of a diethanolamine resin anchor that facilitates boronic acid immobilization by avoiding the need for exhaustive removal of water in the esterification process. The immobilization of a wide variety of boronic acids onto N,N-diethanolaminomethyl polystyrene (DEAM-PS, 1) can be performed within minutes by simple stirring in anhydrous solvents at room temperature Evidence for the formation of a bicyclic diethanolamine boronate with putative N-B coordination was shown by 1H NMR anal. of DEAM-PS-supported p-tolylboronic acid. The hydrolytic cleavage of the same model boronic acid from the DEAM-PS resin was studied by UV spectroscopy. Hydrolysis and attachment were shown to occur under a rapidly attained equilibrium, and a large excess of water (>32 equiv) is required to effect a practically quant. release of boronic acids from DEAM-PS. Despite their relative sensitivity to water and alcs., DEAM-PS-bound arylboronic acids functionalized with a formyl, a bromomethyl, a carboxyl, or an amino group can be transformed in good to excellent yields into a wide variety of amines, amides, anilides, and ureas, resp. Ugi multicomponent reactions on DEAM-PS-supported aminobenzeneboronic acids, derivatization of multifunctional arylboronic acids, and sequential reactions can also be carried out efficiently. These new DEAM-PS-supported arylboronic acids can be employed directly into resin-to-resin transfer reactions (RRTR). This type of multiresin process helps eliminate time-consuming cleavage and transfer operations, thereby considerably simplifying the outlook of combinatorial library synthesis by manual or automated means. This concept was illustrated by a set of optimized procedures for the Suzuki cross-coupling and the borono-Mannich reactions.
IT 268748-30-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(immobilization of arylboronic acids with diethanolaminomethyl polystyrene, and subsequent reactivity of the polymer supported compds.)
RN 268748-30-7 CAPLUS
CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)- (9CI) (CA INDEX NAME)



RE.CNT 111 THERE ARE 111 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:205428 CAPLUS Full-text
DN 132:347395
TI Resin-to-Resin Suzuki Coupling of Solid Supported Arylboronic Acids
AU Gravel, Michel; Berube, Christian D.; Hall, Dennis G.
CS Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.

SO Journal of Combinatorial Chemistry (2000), 2(3), 228-231
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
OS CASREACT 132:347395
GI

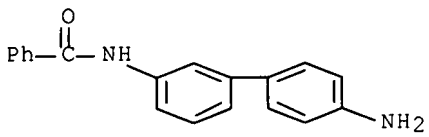


I

AB The first resin-to-resin coupling reaction generating carbon-carbon bonds has been achieved by the palladium-catalyzed Suzuki coupling of di(ethanolamino)methylpolystyrene-bound arylboronic acids with resin-bound iodoarenes to give biaryl derivs. in 55-100% yields upon cleavage of the resin with trifluoroacetic acid in methylene chloride. E.g., resin-bound 3-aminobenzeneboronic acid was treated with 4-chlorobenzoyl chloride to give an resin-bound amide derivative; addition of 0.25 equivalent resin-bound 3-iodobenzylamine and stirring at 105° in DMF in the presence of tetrakis(triphenylphosphine)palladium (0), ethylene glycol, and triethylamine gave a resin-bound aminomethylbiaryl amide which was liberated from the resin with a 1:1 solution of trifluoroacetic acid in methylene chloride to give I in 100% yield. A library of six biaryl derivs. was prepared using the resin-to-resin Suzuki coupling procedure. The resin-to-resin Suzuki coupling procedure allows the preparation of unsym. biaryl derivs. that would be more difficult to prepare on a single solid phase.

IT 268748-30-7P 268748-37-4P 268748-39-6P
268748-41-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of biaryl derivs. by resin-to-resin Suzuki coupling of di(ethanolamino)methylpolystyrene-bound arylboronic acids to resin-bound iodoarenes)

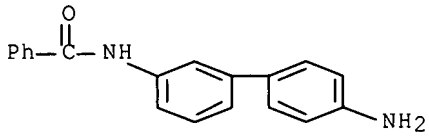
RN 268748-30-7 CAPLUS
CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)- (9CI) (CA INDEX NAME)



RN 268748-37-4 CAPLUS
CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

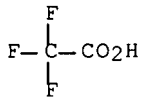
CM 1

CRN 268748-30-7
CMF C19 H16 N2 O



CM 2

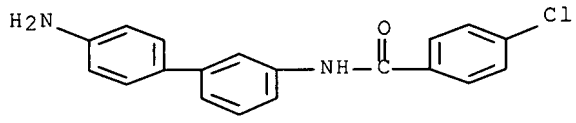
CRN 76-05-1
CMF C2 H F3 O2



RN 268748-39-6 CAPLUS
CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)-4-chloro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

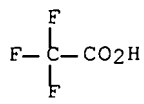
CM 1

CRN 268748-38-5
CMF C19 H15 Cl N2 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

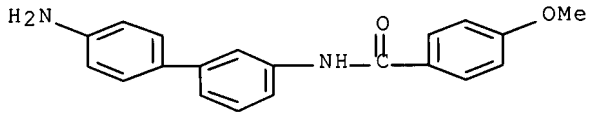


RN 268748-41-0 CAPLUS

CN Benzamide, N-(4'-amino[1,1'-biphenyl]-3-yl)-4-methoxy-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

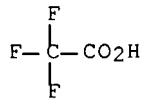
CM 1

CRN 268748-40-9
CMF C20 H18 N2 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2



RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

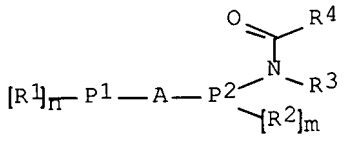
L5 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:596172 CAPLUS Full-text
DN 125:247613
TI Preparation of indolines as 5-HT2B/2C receptor antagonists
IN Gaster, Laramie Mary; Wyman, Paul Adrian; Mulholland, Keith Raymond; Davies, David Thomas; Duckworth, David Malcom; Forbes, Ian Thomson; Jones, Graham Elgin
PA Smithkline Beecham Plc, UK
SO PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9623783	A1	19960808	WO 1996-EP368	19960126 <--
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE				
	CA 2212061	A1	19960808	CA 1996-2212061	19960126 <--
	AU 9646646	A	19960821	AU 1996-46646	19960126 <--
	AU 699727	B2	19981210		
	BR 9607016	A	19971028	BR 1996-7016	19960126 <--

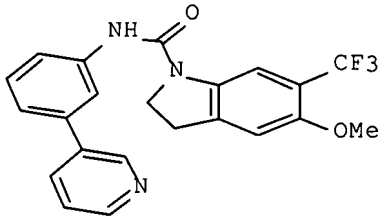
	EP 808312	A1	19971126	EP 1996-902259	19960126 <--
	EP 808312	B1	20001102		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI				
	CN 1179156	A	19980415	CN 1996-192777	19960126 <--
	JP 10513442	T	19981222	JP 1996-523247	19960126 <--
	HU 9901115	A2	19990728	HU 1999-1115	19960126 <--
	HU 9901115	A3	20000228		
	RO 115522	B3	20000330	RO 1997-1439	19960126 <--
	AT 197300	T	20001115	AT 1996-902259	19960126 <--
	ES 2151652	T3	20010101	ES 1996-902259	19960126 <--
	PT 808312	T	20010330	PT 1996-902259	19960126 <--
	PL 184490	B1	20021129	PL 1996-321706	19960126 <--
	CZ 294097	B6	20041013	CZ 1997-2445	19960126
	ZA 9600758	D	19970930	ZA 1996-758	19960131 <--
	IL 116998	A	20010808	IL 1996-116998	19960201 <--
	IN 1996DE00234	A	20050311	IN 1996-DE234	19960202
	FI 9703205	A	19971001	FI 1997-3205	19970801 <--
	NO 9703543	A	19971001	NO 1997-3543	19970801 <--
	NO 313520	B1	20021014		
	US 5990133	A	19991123	US 1997-875506	19971016 <--
	HK 1003883	A1	20010831	HK 1998-103018	19980409 <--
	US 6235758	B1	20010522	US 1999-359606	19990723 <--
	GR 3035075	T3	20010330	GR 2000-402763	20001213 <--
	US 2003105139	A1	20030605	US 2001-767245	20010122 <--
	US 6638953	B2	20031028		
PRAI	GB 1995-2052	A	19950202		
	GB 1995-8327	A	19950425		
	GB 1995-8967	A	19950503		
	GB 1995-16845	A	19950817		
	GB 1995-17542	A	19950826		
	GB 1995-18574	A	19950912		
	WO 1996-EP368	W	19960126		
	US 1997-875506	A3	19971016		
	US 1999-359606	A3	19990723		

OS CASREACT 125:247613; MARPAT 125:247613

GI



I



II

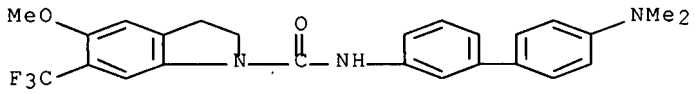
AB The title compds. [I; P1, P2 = Ph, aromatic or partially saturated monocyclic or bicyclic heterocyclic ring; A = bond, (substituted) C1-5 alkylene, etc.; R1, R2 = H, (substituted) C1-6 alkyl, C2-6 alkenyl, etc.; R3 = H, C1-6 alkyl; R4 = 1-indolinyl, etc.; n, m = 0-2], useful in the treatment of CNS disorders such as anxiety, were prepared Thus, treatment of 3-(3-pyridyl)aniline with 1,1-dicarbonyldiimidazole in CH2Cl2 followed by reaction of the intermediate

with 5-methoxy-6-trifluoromethylindoline in DMF afforded 85% the indoline II which showed pKi of 5.8-9.7 against [3H]-mesulergine binding to rat or human 5-HT2C clones expressed in 293 cells in vitro.

IT 181631-21-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of indolines as 5-HT2B/2C receptor antagonists)

RN 181631-21-0 CAPLUS

CN 1H-Indole-1-carboxamide, N-[4'-(dimethylamino)[1,1'-biphenyl]-3-yl]-2,3-dihydro-5-methoxy-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:543429 CAPLUS Full-text

DN 122:267113

TI Polyamide and amide compound compositions with good degree of crystallinity

IN Kitagawa, Hiroshi; Yana, Yoshitaka; Mizoguchi, Kazuaki; Kawahara, Yasuyuki; Sadamitsu, Kyoshi; Yoshimura, Masafumi; Ikeda, Naoki

PA Shin Nippon Rika KK, Japan; New Japan Chemical Co., Ltd.

SO Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06271762	A	19940927	JP 1994-15830	19940113 <--
	JP 3477787	B2	20031210		
	JP 2004035895	A	20040205	JP 2003-290992	20030811
PRAI	JP 1993-26179	A	19930120		
	JP 1994-15830	A3	19940113		

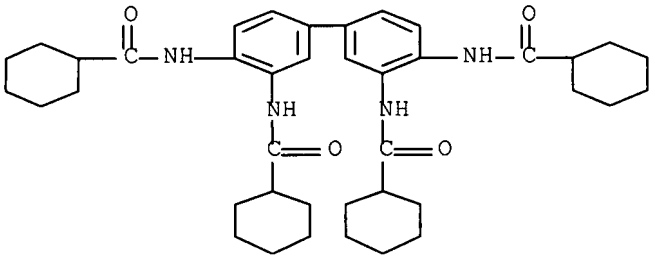
OS MARPAT 122:267113

AB The compns. comprise a polyamide and a compound selected from polycarboxylic acid amide, polyamine polyamide and/or polyamino amide. A composition from nylon 6 containing 0.2 phr N,N'-dicyclohexylterephthalamide showed degree of crystallinity 182°.

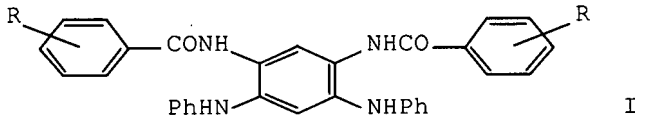
IT 162957-57-5
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(polyamide and amide compound compns. with good degree of crystallinity)

RN 162957-57-5 CAPLUS

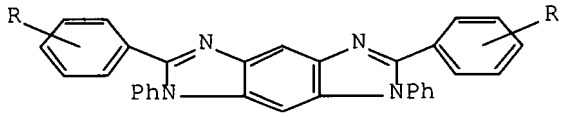
CN Cyclohexanecarboxamide, N,N',N'',N'''-[1,1'-biphenyl]-3,3',4,4'-tetrayltetrakis- (9CI) (CA INDEX NAME)



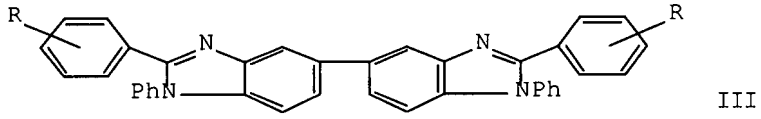
L5 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1978:152492 CAPLUS Full-text
DN 88:152492
TI Synthesis and study of new heterocyclic diamines
AU Korshak, V. V.; Rusanov, A. L.; Batirov, I.; Tugushi, D. S.; Kalontarov, I. Ya.
CS Inst. Elementoorg. Soedin., Moscow, USSR
SO Doklady Akademii Nauk Tadzhikskoi SSR (1977), 20(9), 26-8
CODEN: DANTAL; ISSN: 0002-3469
DT Journal
LA Russian
OS CASREACT 88:152492
GI



I

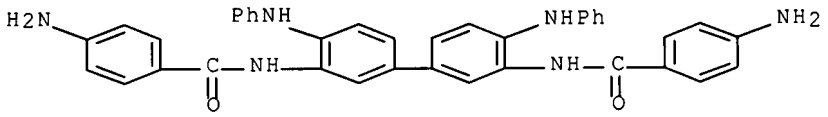


II

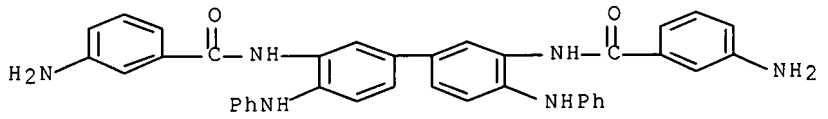


III

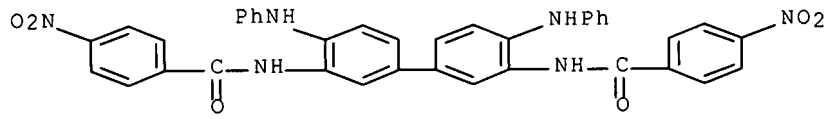
AB Phenylenebisbenzamides I (R = o-, m-O2N), prepared by acylation of a benzenetetramine with RC6H4COCl, were cyclodehydrated to give benzodiimidazoles II which were hydrogenated to give II (R = o-, m-H2N). Hydrogenation of I gave the amines which were cyclodehydrated to give the identical II. Analogously obtained were bisbenzimidazoles III (R = o-, m-H2N) and their nitro intermediates III (R = o-, m-O2N).
IT 66159-48-6P 66159-49-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclodehydration of)
RN 66159-48-6 CAPLUS
CN Benzamide, N,N'-[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]bis[4-amino- (9CI) (CA INDEX NAME)



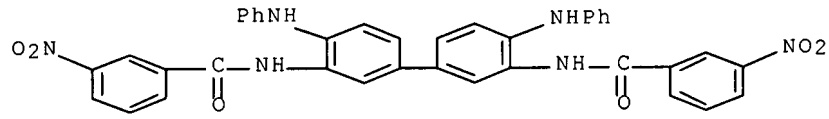
RN 66159-49-7 CAPLUS
CN Benzamide, N,N'-[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]bis[3-amino- (9CI) (CA INDEX NAME)



IT 65847-17-8P 65847-18-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, cyclodehydration, and hydrogenation of)
RN 65847-17-8 CAPLUS
CN Benzamide, N,N'-[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]bis[4-nitro- (9CI) (CA INDEX NAME)



RN 65847-18-9 CAPLUS
CN Benzamide, N,N'-[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]bis[3-nitro- (9CI) (CA INDEX NAME)



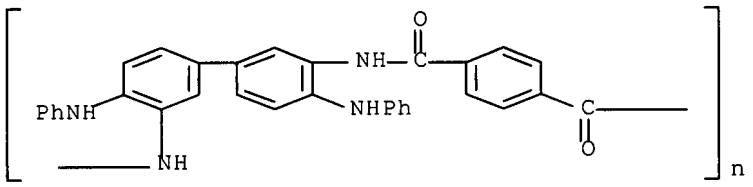
L5 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1975:514987 CAPLUS Full-text
DN 83:114987
TI Preparation of formic acid-soluble poly(N-phenylbenzimidazoles)
AU Pravednikov, N.; Voznesenskaya, N. N.; Berendyaev, V. I.; Kotov, B. V.
CS L. Ya Karpov Inst. Phys. Chem., Moscow, USSR
SO Plaste und Kautschuk (1975), 22(6), 476-7
CODEN: PLKAAM; ISSN: 0048-4350
DT Journal
LA German

AB 1,3-Diamino-4,6-dianilinobenzene and 3,3'-diamino-4,4'-dianilinobiphenyl were copolymd. with iso- and terephthaloyl chloride and with 4,4'-oxybis(benzoyl chloride) in sulfolane containing amide HCl acceptors to provide poly(anilino amides) which were cyclized in vacuo at 300-70° to give heat-resistant, dielec. poly (N- phenylbenzimidazoles) soluble in 85% HCO2H. Cyclized diaminodianilinobenzene- terephthaloyl chloride polymer [31497-74-2] of logarithmic viscosity (0.5% in 85% HCO2H at 25°) 1.4 was 18-20% soluble in 85% HCO2H, was stable in air to 450°, resisted 30% KOH for 12 hr, and had dielec. permeability and dielec. loss tangent 4.5 and 4.1+10-3, resp. (at 20° and 1 kH2) elec. breakdown resistance 230 kV/mm, log(sp. resistance) 14.51 at 180° and >1012 Ω-cm sp. resistance at 300°, tensile strength 1400 kg/cm2, and elongation 10%.

IT 39820-26-3P 39820-29-6P 40514-06-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

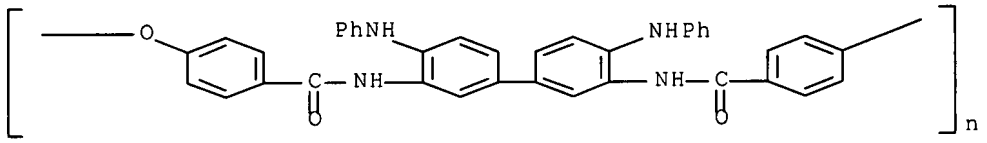
RN 39820-26-3 CAPLUS

CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,4-phenylenecarbonyl] (9CI) (CA INDEX NAME)



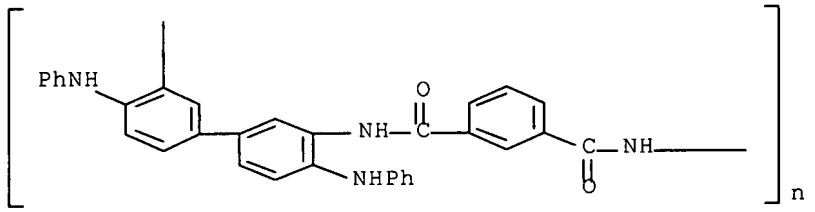
RN 39820-29-6 CAPLUS

CN Poly[oxy-1,4-phenylenecarbonylimino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,4-phenylene] (9CI) (CA INDEX NAME)

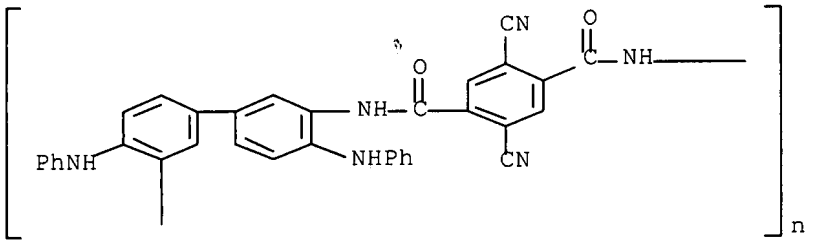


RN 40514-06-5 CAPLUS

CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,3-phenylenecarbonyl] (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1975:58433 CAPLUS Full-text
DN 82:58433
TI Synthesis and thermal cyclotransformations of o-substituted polyiminoimides
AU Vasil'eva, I. V.; Teleshov, E. N.; Yarosh, V. N.; Berendyaev, V. I.; Voznesenskaya, N. N.; Kotov, B. V.; Pravednikov, A. N.
CS Nauchno-Issled. Fiz.-Khim. Inst. im. Karpova, Moscow, USSR
SO Vysokomolekulyarnye Soedineniya, Seriya B: Kratkie Soobshcheniya (1974), 16(10), 779-83
CODEN: VYSBAI; ISSN: 0507-5483
DT Journal
LA Russian
GI For diagram(s), see printed CA Issue.
AB The ortho-substituted polyamides I (Z = direct bond, SO2, O; R = NHPh, OH) and II were converted to the corresponding CN-containing polybenzimidazoles (PBI) and polybenzoxazoles (PBO) on heating. In the first case the reaction was nearly completely shifted to the side of PBI formation, but the formation of PBO was complicated by side reacions. The conversion mechanism apparently included a shift in the reaction equilibrium from isomerization cyclization to the side of polycyanamide formation with subsequent irreversible dehydrocyclization and imidazole and benzoxazole ring formation. Model compds. for investigating the conversions were prepared
IT 54190-54-4
RL: USES (Uses)
(isomerization and ring formation in, by heat, mechanism of)
RN 54190-54-4 CAPLUS
CN Poly[iminocarbonyl(2,5-dicyano-1,4-phenylene)carbonylimino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]] (9CI) (CA INDEX NAME)

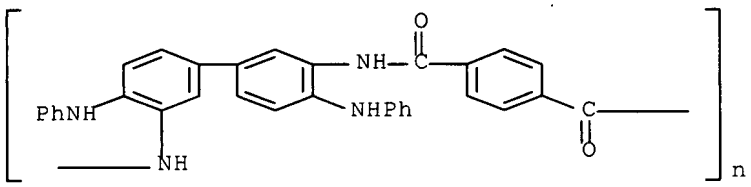


L5 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1974:491978 CAPLUS Full-text
DN 81:91978
TI Synthesis and properties of poly(N-phenylbenzimidazoles)
AU Voznesenskaya, N. N.; Berendyaev, V. I.; Kotov, B. V.; Voishchev, V. S.; Pravednikov, A. N.
CS Nauchno-Issled. Fiz.-Khim. Inst. im. Karpova, Moscow, USSR
SO Vysokomolekulyarnye Soedineniya, Seriya B: Kratkie Soobshcheniya (1974), 16(2), 114-16
CODEN: VYSBAI; ISSN: 0507-5483
DT Journal
LA Russian
AB Poly-o-anilinoamide prepolymers for polybenzimidazoles (PBI) were prepared by the cyclodehydration (in vacuum at 300-370.deg.) in tetramethylene sulfone of aromatic acid chlorides and N-(aminophenyl)anilines [I, R = NH2, H; R1 = NH2, H; R2 = NH2, 2-NHC6H3NH2, 3,4-H2N(PhNH)C6H3, 4-(o-H2NC6H4NH)C6H4; R3 = NHPh,

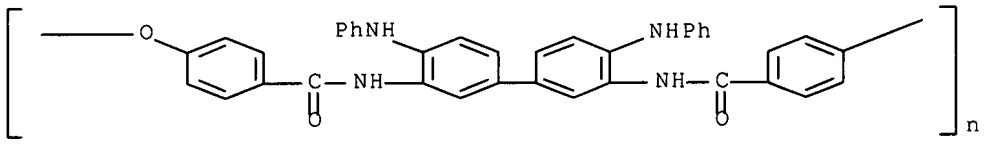
H]. Such polyanilinoamides had higher mol. weight than when prepared in N-methylpyrrolidone and gave HCO2H- and H2SO4-soluble PBI which formed heat-stable films (weight loss began at 450-500.deg.). The films also had good mech. and dielec. properties. The PBI from 1,3-diamino-4,6-dianilinobenzene-terephthaloyl chloride copolymer [26615-84-9] had sp. resistance >1012 ohm cm at 300.deg..

IT 39820-26-3P 39820-29-6P 40514-06-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and viscosimetric properties of)

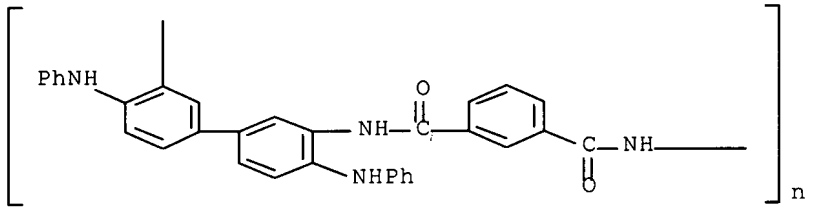
RN 39820-26-3 CAPLUS
CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,4-phenylenecarbonyl] (9CI) (CA INDEX NAME)



RN 39820-29-6 CAPLUS
CN Poly[oxy-1,4-phenylenecarbonylimino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,4-phenylene] (9CI) (CA INDEX NAME)



RN 40514-06-5 CAPLUS
CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,3-phenylenecarbonyl] (9CI) (CA INDEX NAME)



L5 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1974:478937 CAPLUS Full-text
DN 81:78937
TI Semipermeable membranes
IN Hoehn, Harvey; Richter, John Williams
PA du Pont de Nemours, E. I., and Co.
SO Ger. Offen., 107 pp.

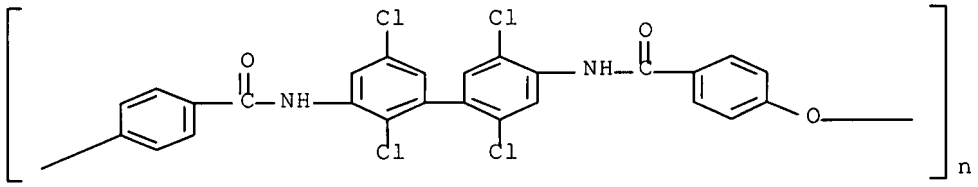
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2336870	A1	19740131	DE 1973-2336870	19730719 <--
	DE 2336870	C2	19830505		
	US 3822202	A	19740702	US 1972-303210	19721102 <--
	US 3899309	A	19750812	US 1973-322800	19730111 <--
	FR 2193634	A1	19740222	FR 1973-26510	19730719 <--
	FR 2193634	B1	19800328		
	JP 50099971	A	19750808	JP 1973-82445	19730719 <--
	JP 55041802	B	19801027		
	GB 1435152	A	19760512	GB 1973-34398	19730719 <--
	GB 1435153	A	19760512	GB 1975-30990	19730719 <--
	US 30351	E	19800729	US 1976-687639	19760518 <--
PRAI	US 1972-273802	A	19720720		
	US 1972-303210	A	19721102		
	US 1973-322800	A	19730111		

AB Membranes useful in the separation of gases by diffusion contain .geq. 50% aromatic polyamide, polyester, or polyimide, the chain rotation of which is sterically hindered. Thus, a 16% C2H2Cl4 solution of isophthaloyl chloride-4,4'-isopropylidenebis(2,6-dichlorophenol) polymer [29964-00-9] is coated to 0.38 mm on a PTFE wax-coated glass plate and heated 15 min at 110.deg. to give a 38 μ semipermeable membrane showing a diffusion selectivity for oxygen [7782-44-7] over nitrogen [7727-37-9] of 5.6:1.

IT 52233-79-1
RL: USES (Uses)
(semipermeable membranes, for gas separation by diffusion)

RN 52233-79-1 CAPLUS
CN Poly[oxy-1,4-phenylenecarbonylimino(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)iminocarbonyl-1,4-phenylene] (9CI) (CA INDEX NAME)



L5 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1973:526839 CAPLUS Full-text
DN 79:126839
TI Thermodynamics of synthesis of polyheteroarylenes
AU Karyakin, N. V.; Mochalov, A. N.; Sapozhnikov, V. N.; Rabinovich, I. B.
CS USSR
SO Trudy po Khimii i Khimicheskoi Tekhnologii (1972), (2), 134-46
CODEN: TKKTAE; ISSN: 0564-3457
DT Journal
LA Russian

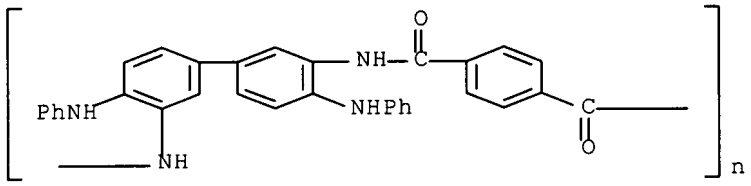
AB The enthalpy(ΔH) of tetramines polycondensation with dianhydrides depends on their resp. basicities and acidities. The polycondensation entropy(ΔS) is neg. and small in comparison with ΔH. The polycondensations of 4,4'-oxydiphthalic anhydride (I) [1823-59-2] with bis(3,4-diaminophenyl) sulfone

[13224-79-8], bis(3,4-diaminophenyl) ketone [5007-67-0], 3,3',4,4'-tetraminobiphenyl [91-95-2], bis(3,4- diaminophenoxy)benzene [42376-72-7], bis(3,4-diaminophenoxy)methane [42437-53-6], 1,3-diamino-4,6-dianilinobenzene [4608-07-5], 3,3'-diamino-4,4'-dianilinobiphenyl [18888-98-7], or bis(3-amino-4- anilinophenyl) sulfone [25351-68-2], and the polycondensations of 3,3',4,4'-tetraminodiphenyl ether [2676-59-7], with I, pyromellitic dianhydride [89-32-7], 4,4'-diphthalic anhydride ketone [2421-28-5], or 4,4'-diphthalic anhydride sulfone [2540-99-0] in solns. proceed nearly to completion. The ΔH of these reactions vary considerably despite their similarity. This is because the reactions involve not only the polycondensations, but also the energy of desolvation and the energy of the partial ionization of CO2H and NH2 groups in the linear poly(amide amino acids) (II). The intramol. cyclodehydration of II proceeds in 2 stages giving III and IV. The formation of IV is favored thermodynamically even at room temperature, but due to kinetic factors I .far. IV reaction occurs only above the temperature at which I become viscoelastic.

IT 39820-26-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, thermodn. of)

RN 39820-26-3 CAPLUS

CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,4-phenylenecarbonyl] (9CI) (CA INDEX NAME)



L5 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1973:72645 CAPLUS Full-text

DN 78:72645

TI Two-stage synthesis of poly(N-phenylbenzimidazoles)

AU Korshak, V. V.; Rusanov, A. L.; Tugushi, D. S.; Cherkasova, G. M.

CS Inst. Elementoorg. Compds., Moscow, USSR

SO Macromolecules (1972), 5(6), 807-12
CODEN: MAMOBX; ISSN: 0024-9297

DT Journal

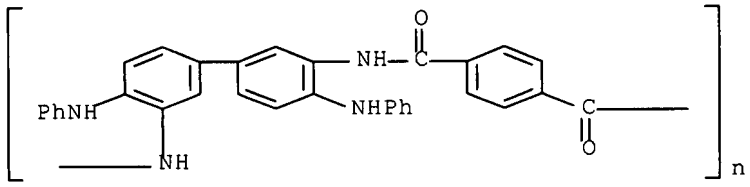
LA English

AB The low-temperature solution polymerization of 1,3-diamino-4,6-dianilinobenzene (I), 3,3'-diamino-4,4'-dianilinobiphenyl, and 3,3'-diamino-4,4'- dianilinodiphenyl sulfone with various dicarboxylic acid dichlorides gave high-mol.-weight poly(o-anilino amides), which were cyclized at 300-310.deg. to poly(N-phenylbenzimidazoles), which were soluble in HCOOH and tetrachloroethane-PhOH and formed strong films. For example, I and terephthaloyl chloride gave poly[imino(4,6-dianilino-m-phenylene)iminoterephthalyl] (II) [31497-73-1], which was cyclized to poly[(1,7-dihydro-1,7-diphenylbenzo[1,2-d:4,5-d']diimidazole-2,6-diyl)-p-phenylene] (III) [31497-74-2]. Twenty analogous polyamides and their corresponding polybenzimidazoles were also prepared, and dynamic and isothermal thermogravimetric anal. curves for 7 of the polybenzimidazoles were given and discussed. In addition, 20 model compds. were prepared

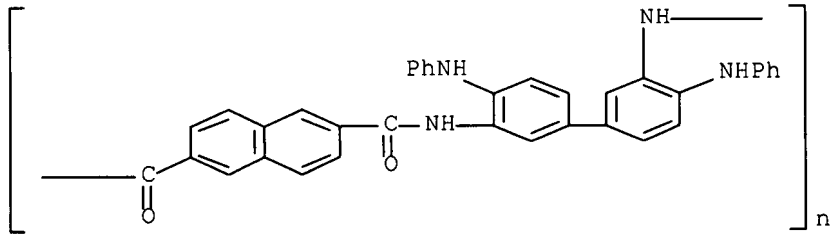
IT 39820-26-3P 39820-27-4P 39820-28-5P
39820-29-6P 39820-30-9P 40514-06-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

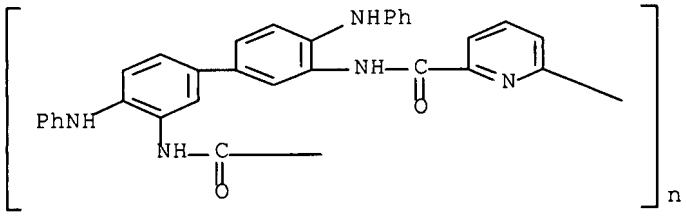
RN 39820-26-3 CAPLUS
CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,4-phenylenecarbonyl] (9CI) (CA INDEX NAME)



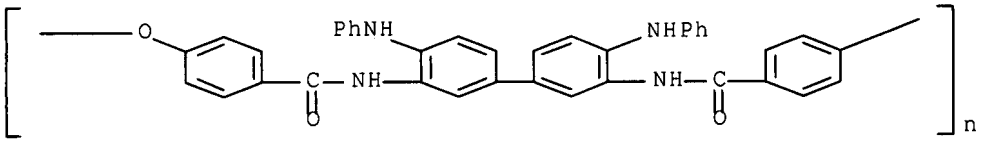
RN 39820-27-4 CAPLUS
CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-2,6-naphthalenediylcarbonyl] (9CI) (CA INDEX NAME)



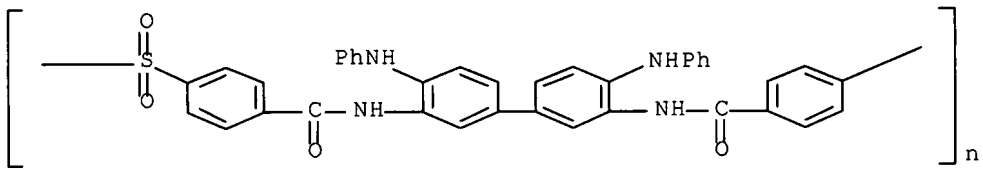
RN 39820-28-5 CAPLUS
CN Poly[2,6-pyridinediylcarbonylimino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl] (9CI) (CA INDEX NAME)



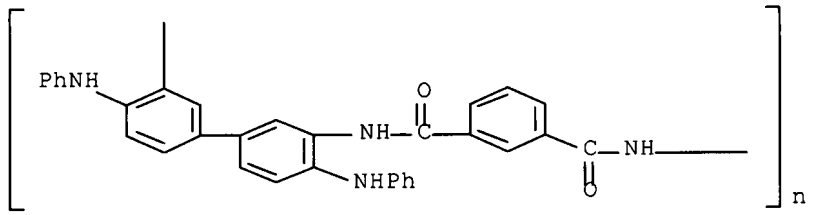
RN 39820-29-6 CAPLUS
CN Poly[oxy-1,4-phenylenecarbonylimino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,4-phenylene] (9CI) (CA INDEX NAME)



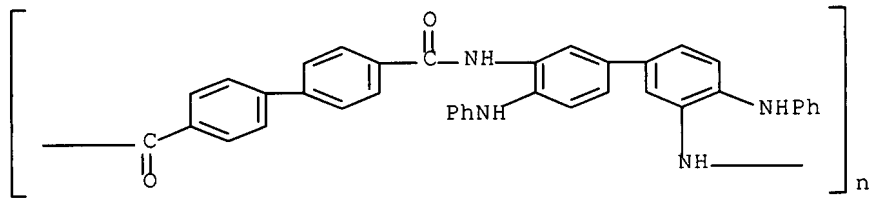
RN 39820-30-9 CAPLUS
CN Poly[sulfonyl-1,4-phenylenecarbonylimino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,4-phenylene] (9CI) (CA INDEX NAME)



RN 40514-06-5 CAPLUS
CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl-1,3-phenylenecarbonyl] (9CI) (CA INDEX NAME)

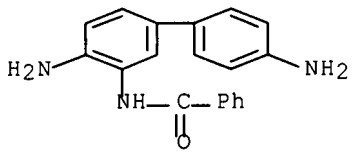


IT 40514-07-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40514-07-6 CAPLUS
CN Poly[imino[4,4'-bis(phenylamino)[1,1'-biphenyl]-3,3'-diyl]iminocarbonyl[1,1'-biphenyl]-4,4'-diylcarbonyl] (9CI) (CA INDEX NAME)



L5 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1968:50943 CAPLUS Full-text
DN 68:50943
OREF 68:9899a,9902a
TI Aromatic diazo and azo compounds. LXXIV. Benzidine rearrangement of 2-acylaminohydrazobenzenes. Transacylation of amino groups on an aromatic ring
AU Rakusan, J.; Allan, Zdenek J.
CS Res. Inst. Org. Syn., Pardubice-Rybitvi, Czech.
SO Collection of Czechoslovak Chemical Communications (1967), 32(8), 2882-9
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA German
GI For diagram(s), see printed CA Issue.
AB 2-BzNHC6H4N:NPh (1 g.) was reduced with SnCl2 in 37% HCl at 20° to give I (X = Z = NH2, Y = BzNH) (II), an unknown compound [probably 2,4-H2N(BzNH)C6H3C6H4NH2-4], PhNH2, and 2-BzNHC6H4NH2. II, m. 200° (EtOH), was obtained in 0.4 g. yield by treating the product with aqueous NH3. II heated to 100° in 37% HCl was transacylated to yield .apprx.99% I (X = BzNH, Y = Z = NH2) (III), (the half-period of reaction was 10 min.), identical with III prepared from I (X-BzNH, Y = Z = NO2), m. 212°, by reduction at 20°. Similarly, 2-Ac-NHC6H4N:NPh was reduced and rearranged to I (X = Z = NH2, Y = NHAc) (IV) and analogous by-products. IV was transacylated at 100° in 37% HCl readily and completely to yield I (X = AcNH, Y = Z = NH2) (V) (half-period, .apprx.3 min.), identical with that obtained from I (X = AcNH, Y = Z = NO2). On longer heating 2-methyl-5-(p-aminophenyl)benzimidazole (VI) and a small amount of I (X = Y = Z = NH2) (VII) are formed. On diazotization II, III, IV, V and VI all form 5-(p-diazoniumphenyl)benzotriazole. 2,4-(H2N)2C6H3NHAc heated at 100° in aqueous HCl produces 2-methyl-5-aminobenzimidazole (VII) and a small amount of 2,5-(H2N)C6H3NHAc (IX). IX treated in this way gives only VIII. All identifications were carried out by paper chromatog using 4-Me2NC6H4CHO as indicator.
IT 17716-44-8P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from 3'-(phenylazo)benzanilide, and transacylation of)
RN 17716-44-8 CAPLUS
CN Benzanilide, 2'-amino-5'-(p-aminophenyl)- (8CI) (CA INDEX NAME)



L5 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1958:45297 CAPLUS Full-text
DN 52:45297
OREF 52:8079d-i,8080a-e
TI Quinone imides. XLV. Structures of aromatic amine adducts of p-benzoquinonedibenzimide
AU Adams, Roger; Werbel, Leslie M.
CS Univ. of Illinois, Urbana
SO Journal of Organic Chemistry (1957), 22, 1287-91
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable

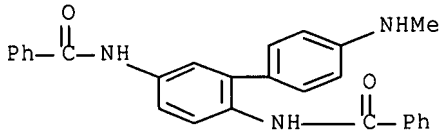
AB cf. C.A. 51, 17803f. A study was made of the structures of products obtained by the addition of aromatic and alicyclic amines and of aromatic hydrocarbons in the presence of anhydrous AlCl3 to quinone diimides. The adduct of C6H6 and p-(PhSO2NH)2C6H4 (I) was shown to be 2,5-dibenzenesulfonamidobiphenyl (II) by an unequivocal synthesis. Yellow fuming HNO3(25 ml.), 25 ml. H2O, and 2.5 g. 2-p-toluenesulfonamidobiphenyl warmed on a steam bath 13 hrs. and the powdered cold yellow product filtered off gave 1.5 g. 5,2-O2N(p-MeC6H4SO2NH)C6H3Ph, m. 170-2° (AcOH). The nitro compound (1 g.), 2 g. PhOH, and 15 ml. com. 48% HBr refluxed 1.5 hrs. and the cooled mixture poured into 100 ml. H2O, the solution made basic with 15% aqueous NaOH, and filtered gave 0.32 g. 2,5-H2N(O2N)C6H3Ph (III), m. 124-5.5° (alc.). III (1 g.) in 20 ml. absolute MeOH and 0.5 g. Raney Ni slurry in H2O stirred with dropwise addition of 0.3 g. 100% N2H4.H2O in 8 ml. MeOH and the mixture refluxed 45 min. on a steam bath, the filtered solution evaporated and the dark purple liquid residue taken up in 25 ml. C5H5N, treated with 3.3 g. PhSO2Cl, the cooled mixture poured into iced HCl and filtered, the pink residue dried, and the crude diamide (1.87 g., m. 189-91°) recrystd. 3 times from alc. gave II, m. 202-3°. The constitutions of the piperidine and morpholine adducts of p-(BzNH)2C6H4 (Ia) were similarly determined and that of the aniline adduct was established by comparison of its Bz derivative with a compound (IV) synthesized by an unequivocal route. MeOH containing 0.2 g. p-H2NC6H4(p-O2NC6H4)NH treated with 0.1 ml. 100% N2H4.H2O and a pinch of Raney Ni and the mixture warmed 1 hr. on the steam bath, the filtered solution evaporated and the residue refluxed 4 hrs. in C5H5N with 0.3 ml. BzCl, the cooled solution poured onto iced HCl, and the product recrystd. from alc. gave IV, N,N',N''-tribenzoyl-4,4'-diaminodiphenylamine, m. 310-12°. The adduct of PhNH2 and Ia (C.A. 47, 6893h) (0.2 g.) in C5H5N and 0.1 ml. BzCl warmed 1 hr. on the steam bath and poured into iced HCl yielded 95% IV. BzCl (4.9 g.) and 5.3 g. 3,4-Cl(O2N)C6H3NH2 in C5H5N warmed 3 hrs. at 100° and the cooled mixture poured into iced HCl gave 7.85 g. 3,4-R(O2N)C6H3NHBz (V) (R = Cl) (Va), m. 163-4° (alc.). Va (1.9 g.) and 25 ml. PhNH2 (redistd. over Zn dust) heated 3 hrs. at 185° (N atmospheric) and the cooled mixture poured into 100 ml. H2O, freed from excess PhNH2 by steam distillation and the cooled residue filtered, the dark orange solid treated with 25 ml. alc., and the orange solid (1.2 g.) recrystd. from alc. gave V (R = PhNH) (Vb), m. 216.5-18°. Vb (0.4 g.) in 75 ml. MeOH treated with a small amount of Raney Ni and 0.4 ml. 100% N2H4.H2O and the mixture heated 1 hr. at 100°, the filtered solution evaporated and the gum by-product heated 1 hr. at 100° with 0.2 ml. BzCl, the cooled solution poured into a slurry of ice and HCl, and filtered gave 0.3 g. 2-substituted-p-phenylenedibenzamide (VI) (substituent = R = PhNH), m. 248-9°, not identical with the adduct of PhNH2 and I. Va (0.7 g.) and 2 ml. morpholine refluxed 1.5 hrs. and the cooled mixture poured into ice H2O gave 0.83 g. V (R = morpholino)(Vc), m. 150-1.5° (dilute alc.). Vc (0.25 g.) in 15 ml. MeOH treated with a small amount of Raney Ni and 1 ml. 100% N2H4.H2O and the hot mixture heated 25 min. at 100°, the filtered solution evaporated and the residue benzoylated in C5H5N with 0.3 ml. BzCl by heating the mixture 1.5 hrs. at 100°, the cooled mixture poured into ice and HCl, and the solid recrystd. from dilute alc. gave 0.2 g. VI (R = morpholino), m. 213.5-4.5°. Similarly was obtained a 78.5% yield of V (R = piperidino), m. 117.5-18.5° (C6H6-C6H12), converted as above to VI (R = piperidino), m. 180-1° (dilute alc.). Proof of the structure of the PhNH2 adduct of Ia furnished a 2nd example of 1,6-addition to p-benzoquinone diimides. Adducts of PhNMe2 and PhNHMe with Ia were assumed to have structures similar to those postulated for the analogous adducts with I as determined by conversion of the PhNHMe adducts to PhNMe2 adducts by methylation with MeI in HCONMe2 (C.A. 48, 12020b). Ia (2 g.) in 20 ml. CHCl3 and 0.69 g. redistd. PhNHMe in 20 ml. CHCl3 kept 24 hrs. and poured into 300 ml. ligroine gave VI (R = p-MeNHC6H4) (VIa), m. 209.5-11.5°. Similarly was produced VI (R = p-Me2NC6H4) (VIb), m. 226.5-8.5° (alc.) (micro hot stage), identical with the product obtained by heating 0.5 g. VIa 8 hrs. at 100° with 15 ml. 90% HCO2H and 140 mg. 35% HCHO, pouring the cooled mixture

onto ice, and basifying with 15% NaOH. In contrast to the excellent yields of the single entities VIa and VIb, the adduct of Ia with PhNH2 gave mixts. which were difficult to purify. All the amines added to 1,4-naphthoquinonedibenzenesulfonimide in good yield through the N function and hence no reaction occurred with PhNMe2. An attempt was made to oxidize 2,4-Cl(O2N)C6H3NH2 (VII) with peroxytrifluoroacetic acid. CF3CO2H (65 ml.) refluxed with 5 g. VII and treated dropwise in 30 min. with 17.3 ml. 30% H2O2, the deep red solution refluxed 1 hr. and the cooled solution poured into ice H2O, filtered, and dried gave 4.0 g. orange solid. The solid (1 g.) extracted with ligroine and the extract evaporated yielded 2,1,4-Cl(O2N)2C6H3 (VIII), m. 57-9°. The red insol. material (0.17 g.), m. 280-1° (C6H6), appeared to be a triphenylamine derivative formed by condensation of 1 mole VII with 2 moles VIII.

IT 118044-91-0P, Benzamide, N,N'-[(p-methylaminophenyl)-p-phenylene]bis- 122095-40-3P, Benzamide, N,N'-[(p-dimethylaminophenyl)-p-phenylene]bis-
RL: PREP (Preparation)
(preparation of)

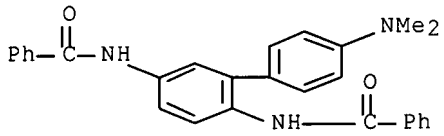
RN 118044-91-0 CAPLUS

CN Benzamide, N,N'-[(p-methylaminophenyl)-p-phenylene]bis- (6CI) (CA INDEX NAME)



RN 122095-40-3 CAPLUS

CN Benzamide, N,N'-[(p-dimethylaminophenyl)-p-phenylene]bis- (6CI) (CA INDEX NAME)



L5 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1956:71823 CAPLUS Full-text

DN 50:71823

OREF 50:13449d

TI Acid amide derivatives of azo dyes

IN Schmid, Max; Moser, Eduard; Danuser, Jakob; Mory, Rudolf; Mueller, Willy; Wuergler, Jakob

PA C I B A Ltd.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2741656		19560410	US 1952-273364	19520225 <--

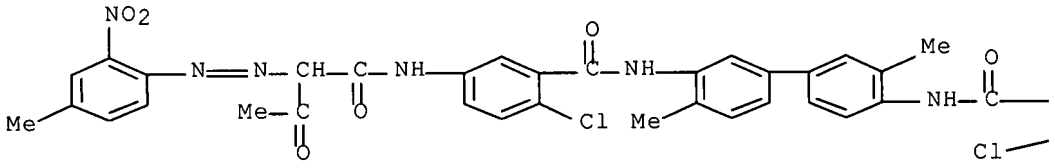
AB See Brit. 730,384 (C.A. 50, 10418a).

IT 873404-24-1P, 4',4'''-Bi-o-benzotoluidide, 2,2''-dichloro-5,5''-bis[2-(2-nitro-p-tolylazo]acetoacetamido]- 873404-25-2P, 4',4'''-Bi-o-benzotoluidide, 4,4''-bis(-2-hydroxy-1-naphthylazo)- 873404-26-3P, 4',4'''-Bi-o-benzotoluidide, 4,4''-bis[1-[(4-chloro-2,5-dimethoxyphenyl)carbamoyl]acetonylazo]-
RL: PREP (Preparation)
(preparation of)

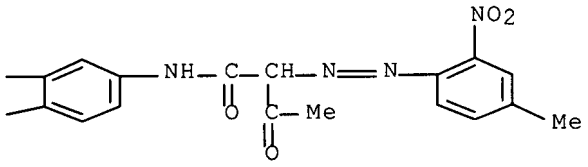
RN 873404-24-1 CAPLUS

CN 4',4'''-Bi-o-benzotoluidide, 2,2''-dichloro-5,5''-bis[2-(2-nitro-p-tolylazo]acetoacetamido]- (5CI) (CA INDEX NAME)

PAGE 1-A

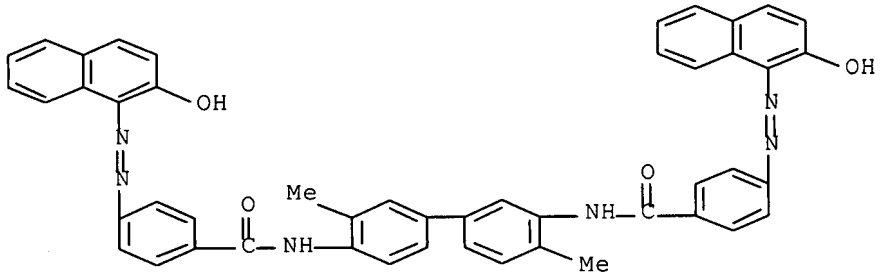


PAGE 1-B



RN 873404-25-2 CAPLUS

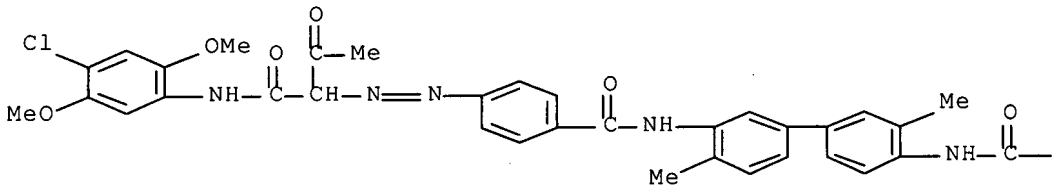
CN 4',4'''-Bi-o-benzotoluidide, 4,4''-bis(-2-hydroxy-1-naphthylazo)- (5CI) (CA INDEX NAME)



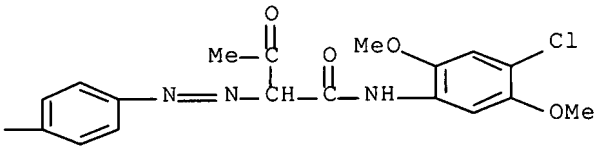
RN 873404-26-3 CAPLUS

CN 4',4'''-Bi-o-benzotoluidide, 4,4''-bis[1-[(4-chloro-2,5-dimethoxyphenyl)carbamoyl]acetonylazo]- (5CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L5 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1956:71822 CAPLUS Full-text
DN 50:71822
OREF 50:13448i,13449a-d
TI Azo dyes
IN Rath, Hermann; Feess, Erich
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 880775		19530625	DE 1951-R5826	19510426 <--

AB Textile fibers, such as cellulose, wool, protein, polyamide, or similar alkali-sensitive fibers, are bottomed with a water-soluble derivative (I) of a N-aryl-o-hydroxyaroylamide, such as an acetal, glucoside, or sulfate thereof, coupling is effected on the fiber with an aromatic diazo compound, and the solubilizing residue of I is split off before coupling by means of an acid or enzymically, or during coupling by addition of NH3 or of a bicarbonate. A suitable manner of preparing I comprises dropping ClSO3H 10 cc. into a suspension of 2,3-HOC10H6CONHPh (II) 15 g. in PhN(Me)2 60 cc. cooled below 10°, heating the mixture with agitating 0.5 h. at 60-5°, cooling, adding a solution of KOH 30 g. in water 30 cc., and stirring until a thick salt mass (III) is precipitated and the liquid phase is separated into 2 layers. III, isolated by sucking off and recrystd. from AmOH or water, gives the K salt (IV) of the sulfated II. Similarly II 7 g. suspended in quinoline 10 cc. is treated with agitation with acetobromoglucose 10 g. and Ag oxide 5 g., stirring continued 2 h., the pasty mass dissolved in warm glacial AcOH, the solution triturated with ice water, and the resulting tetraacetate deacylated by a catalytic ester interchange with MeONa in MeOH to give the glucoside (V) of II which can be purified by recrystn. from water. Wool is bottomed with a hot aqueous 0.3% IV or V solution, H2SO4 1% based on the wool weight (or p-MeC6H4SO3H 1% or HCOOH 3%) added, bottoming continued a short period, the wool squeezed off, treated with dilute NH4OH to neutralize the acid, squeezed off once more, impregnated with a solution of diazotized 1,2,4-H2N(Me)ClC6H3, and finished in the usual way. A red dyeing is obtained. Splitting off of the solubilizing radical (and therewith fixing of II on the fiber) can also be effected by treating the bottomed wool with an aqueous solution of emulsion or

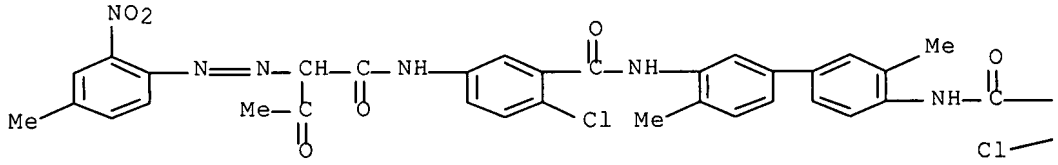
taka-diastase. A diazo salt solution containing an alkali metal bicarbonate, NH3, or pyridine can be used to develop the shade whereby coupling and removal of the solubilizing radical takes place in a single step.

IT 873404-24-1P, 4',4'''-Bi-o-benzotoluidide, 2,2''-dichloro-5,5''-bis[2-(2-nitro-p-tolylazo]acetoacetamido]- 873404-25-2P, 4',4'''-Bi-o-benzotoluidide, 4,4''-bis(-2-hydroxy-1-naphthylazo)- 873404-26-3P, 4',4'''-Bi-o-benzotoluidide, 4,4''-bis[1-[(4-chloro-2,5-dimethoxyphenyl)carbamoyl]acetonylazo]-
RL: PREP (Preparation)
(preparation of)

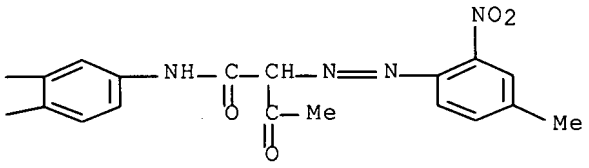
RN 873404-24-1 CAPLUS

CN 4',4'''-Bi-o-benzotoluidide, 2,2''-dichloro-5,5''-bis[2-(2-nitro-p-tolylazo]acetoacetamido]- (5CI) (CA INDEX NAME)

PAGE 1-A

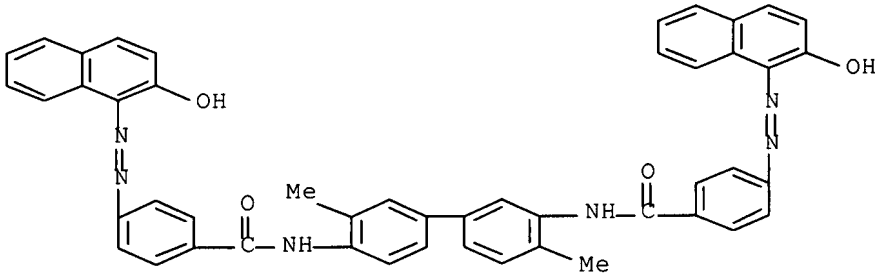


PAGE 1-B



RN 873404-25-2 CAPLUS

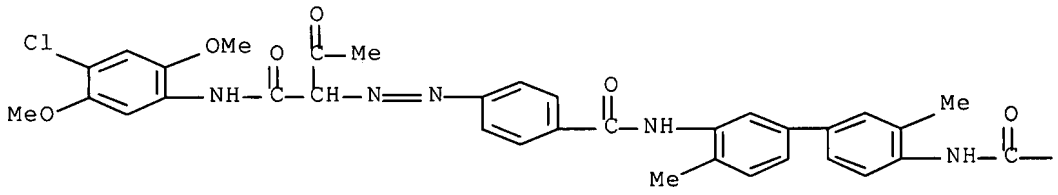
CN 4',4'''-Bi-o-benzotoluidide, 4,4''-bis(-2-hydroxy-1-naphthylazo)- (5CI) (CA INDEX NAME)



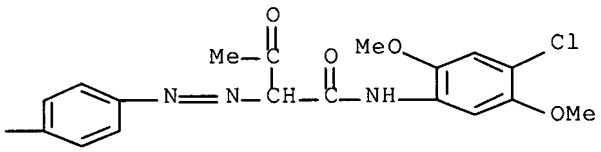
RN 873404-26-3 CAPLUS

CN 4',4'''-Bi-o-benzotoluidide, 4,4''-bis[1-[(4-chloro-2,5-dimethoxyphenyl)carbamoyl]acetonylazo]- (5CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L5 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1956:54585 CAPLUS Full-text
DN 50:54585
OREF 50:10418a-i,10419a-g
TI Acid amide derivatives of azo dyes
PA C I B A Ltd.
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 730384		19550525	GB 1952-5204	19520227 <--

AB Valuable acid amide derivs. of azo dyes are made by treating a cyclic nonvattable amine with a carboxylic acid halide containing at least 1 azo group and an OH group in position ortho to the azo group. Dye 183 from 2,5-H2N(O2N)C6H3OMe and 2,3-HOC10H6CO2H (I) heated with PhCl 3600 while distilling off any H2O, the mixture cooled to about 70°, treated with SOCl2 75 parts, refluxed about 5 h., filtered hot, and cooled, and the crystalline deposit washed with PhCl and dried in vacuo at 60-5° gave 3,4-MeO[2,3-HO(ClOC)C10H5N:N] C6H3OMe (II), dark-bronze, lustrous crystals, m. 253° (decomposition). II 21.5 refluxed 22 h. with dry PhCl 400, pyridine 10 (or NaOAc 5), and [4,3-H2N(Me)C6H3]2 (III) 5.3 filtered hot, and the filter residue washed with hot PhCl about 100 parts and dried in vacuo at 80-90° yielded a dark Bordeaux-red powder (IV), violet-blue in concentrated H2SO4. IV produced a powerful reddish violet color when incorporated in poly(vinyl chloride) (V). Dye 34.0 from diazotized 4,2-Cl(Me)C6H3NH2 and I treated with stirring in C6H6 300 portionwise during 1 h. at 40° with PBr5 48 parts, the mixture stirred 2 h. at 50° and overnight at 20° and filtered, and the filter residue: washed with C6H6 and dried gave the acid bromide, m. 185° (decomposition) (from PhCl). The acid bromide 17.1 in PhCl 120 treated with stirring at 90° with (p-H2NC6H4)2 (VI) 3.68 in PhCl 20 and dry pyridine 5, refluxed 10 h., and filtered hot, and the filter residue washed with hot PhCl and dried gave a dye 17 parts, soft granular red powder, ruby-red in concentrated H2SO4, bluish red in V. A similar dye was obtained by using instead of VI, 1,5-C10H6(NH2)2 31.6 parts; it colored V an even more bluish red tint of very good fastness to migration and light. Finely powdered Na salt 52.1 of the dye from diazotized 4,2,5-Bz(EtO)2C6H2NH2 and I added with

stirring in portions to C6H6 500 and SOCl2 25 parts, the mixture kept 5 h. at 30-5° and filtered, and the residue recrystd. from C6H6 gave the acid chloride, m. 224° (decomposition). The acid chloride 20.7 in PhNO2 200 and dry pyridine 10 heated with stirring to 130°, treated with VI 3.68 in warm PhNO2 20 parts, kept 15 h. at 138-40°, cooled to 80°, and filtered, and the residue washed with a little C6H6 and dried in vacuo as 80° gave a blue pigment, strong blue in V. Azo dye 27.3 from diazotized 4,2,5-BzNH(MeO)(Me)C6H2NH2 and I in o-C6H4Cl2 (VII) 180 heated 1 h. with stirring with SOCl2 13.2, treated slowly with VI 5.52 in VII 30 and dry pyridine 5 parts, heated 15 h. at 130°, and filtered, and the residue washed at 100° with VII and dried in vacuo at 80-90° gave a dye, soft-grained violet powder, violet in V. Azo dye 32.65 from diazotized o-ClC6H4NH2 and I in VII 250 heated 1 h. with stirring with SOCl2 13.2, treated with VI 9.2 in VII 100 parts, heated 5 h. at 120-30°, neutralized with a slow stream of dry NH3, and filtered gave a dye, soft orange powder, pure reddish orange in V. Azo dye 23.4 from diazotized 5,2-Cl(Me)C6H3NH2 and 2-hydroxy-3-anthracenecarboxylic acid in PhCl 180 heated 1 h. at 130° with SOCl2 16.8, treated with VI 5.25 in warm PhCl 30 and pyridine 5 parts, heated 15 h. at 120-30°, and filtered gave a soft-grained powder, pure violet in V. Azo dye 23.2 from diazotized 4,2,5-Cl(MeO)2C6H2NH2 and I, SOCl2 13.2, and III 6.36 parts gave similarly a dye (VIII), fine powder, deep-violet in V. Azo dye 34 from diazotized 3,2-Cl(Me)C6H3NH2 and I in VII 300 rerefluxed 1 h. with SOCl2 15.5, treated with VI 9.2 in VII 90 and dry pyridine 5, stirred 1 h., treated with a solution of the acid chloride from an azo dye 49.9 prepared from 2,5,4-(EtO)2 (BzNH)C6H2NH2 and I, stirred a short time, mixed with VI 9.2 in VII 90 and dry pyridine 10 parts, kept 15 h. at 120°, and filtered gave a violet powder, blue in concentrated H2SO4, strong violet in V. Azo dye 29.2 from p-H2NC6H4CO2H (IX) and 2-C10H7OH (X) boiled in PhCl 500 until all H2O was removed, cooled to about 55°, treated during 15 min. with SOCl2 23.8, heated 1 h. at 80-90°, refluxed 3 days, cooled to 80-90°, treated with III 10.6 in PhCl 200 parts, heated 4 h., and filtered hot gave a dye, fine orange powder, bluish violet in concentrated H2SO4, orange in V. Dye 29.2 from IX and X in C6H6 250 treated during 0.5 h. at room temperature with PCl5 23.0, stirred a few hrs., heated to 40-50°, cooled, and filtered gave 2,1-HOC10H6N: NC6H4COCl-p which was condensed in the usual manner with III 10.6 parts. Dye 35.7 from diazotized o-ClC6H4NH2 and 1-(4-carboxyphenyl)-3-methyl-5-pyrazolone (XI) in C6H6 300 converted with PCl5 23.0 to the acid chloride, and a portion 37.5 condensed in PhCl 800 with III 10.6 parts in the usual manner yielded a yellow powder, yellow in concentrated H2SO4 and in V. Dye 37 from 5,2-Cl(Me)C6H3NH2 and XI in PhCl 500 treated with SOCl2 16.5 and a portion 38.3 of the resulting acid chloride, m. 233-4°, in PhCl 800 treated with bis(4-amino-3-chlorophenyl)methane 13.4 parts gave a yellow powder, yellow-orange in concentrated H2SO4. Dye 33.6 from diazotized IX and 1-(p-methylphenyl)-3-methyl-5-pyrazolone refluxed 6 h. in PhCl 400 and SOCl2 16.5 parts gave the acid chloride, orange powder, m. 176-7°. A portion of the latter 35.5 in PhCl 800 and pyridine 10 refluxed 12 h. with 4,4'-diamino-3,3'-dichlorobiphenyl 12.6 parts gave an orange powder, orange-yellow in concentrated H2SO4, yellow in V. p-AcCH2CONHC6H4CO2H 22.1, m. 174° (prepared from IX and diketene in neutral aqueous solution) dissolved with Na2CO3 5 in H2O 300, treated with crystalline NaOAc 25 and at 5-10° with diazotized 4,2-Me(O2N)C6H3NH2, kept 4 h. at 5-10°, heated to 40-50° during 1 h., and filtered and dried gave an azo dye. A portion of the latter 38.4 in dry PhCl 400 treated at 110° dropwise with stirring with SOCl2 13.8 parts during 15 min., and the mixture refluxed 6-7 h., cooled to 10° and filtered gave 4,2-Me(O2N) C6H3N: NC(:CMeOH)CONHC6H4COClC-p(XII), yellow crystalline powder, m. 245°. III 10.5 in dry PhCl 200 treated with stirring with XII 40.3 parts at 80-5°, and the mixture heated at 110°, cooled to 80°, and filtered gave a greenish yellow dye, yellow in concentrated H2SO4, greenish yellow in V. Dye 41.8, from diazotized IX and 4,2,5-Cl(MeO)2C6H3NHCOCH2Ac in AcOH or weakly alkaline medium, was converted in the usual manner with SOCl2 15 parts to the

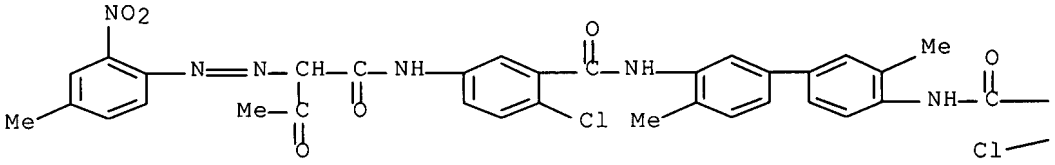
corresponding acid chloride, m. 248-50°. A portion 43.7 in PhCl 600 condensed at 120-30° during 4-5 h. with III 10.6 parts gave a yellow powder, yellow in H2SO4, pure strong yellow in V. 5,2-H2N(Cl)C6H3CO2H condensed with diketene in neutral aqueous medium, the resulting 5,2-AcCH2CONH(Cl)C6H3CO2H coupled with diazotized 4,2-Me(O2N)C6H3NH2, the resulting dye 41.85 treated in PhCl 600 in the usual manner with SOCl2 15, the acid chloride, yellow platelets, m. 204°, 43.7 condensed with III 10.6 in PhCl 800 parts at 120° during 3-4 h., and the precipitate filtered gave a fine yellow powder, yellow in concentrated H2SO4, strong greenish yellow in V. Dye 34, from diazotized 2-methyl-4-chloroaniline and I, treated with SOCl2 15.5 and then condensed with 3-aminopyrene 21.7 parts gave a brown, soft-grained powder, violet in concentrated H2SO4, reddish violet in V. Dye 33.6, from diazotized IX and I, treated with SOCl2 37 and condensed with 2-aminochrysene 42 parts yielded a red-brown, soft-grained powder, violet in concentrated H2SO4, brownish red in V. V 65, dioctyl phthalate 35, and VIII 0.2 parts stirred together and calendered about 3 min. at 140-5° gave a strongly violet-colored foil of good fastness to light and dye migration. The new acid amide derivs. of azo dyes are useful in printing and for coloring hardenable plastics.

IT 873404-24-1P, 4',4'''-Bi-o-benzotoluidide, 2,2''-dichloro-5,5''-bis[2-(2-nitro-p-tolylazo]acetoacetamido]- 873404-25-2P, 4',4'''-Bi-o-benzotoluidide, 4,4''-bis(-2-hydroxy-1-naphthylazo)- 873404-26-3P, 4',4'''-Bi-o-benzotoluidide, 4,4''-bis[1-[(4-chloro-2,5-dimethoxyphenyl)carbamoyl]acetonylazo]-
RL: PREP (Preparation)
(preparation of)

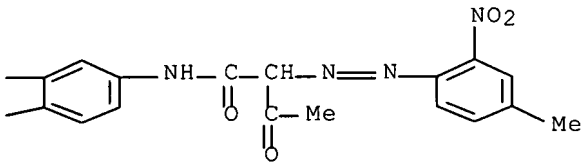
RN 873404-24-1 CAPLUS

CN 4',4'''-Bi-o-benzotoluidide, 2,2''-dichloro-5,5''-bis[2-(2-nitro-p-tolylazo]acetoacetamido]- (5CI) (CA INDEX NAME)

PAGE 1-A

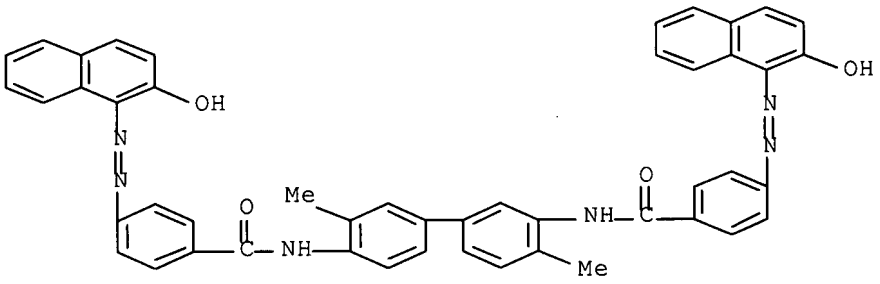


PAGE 1-B



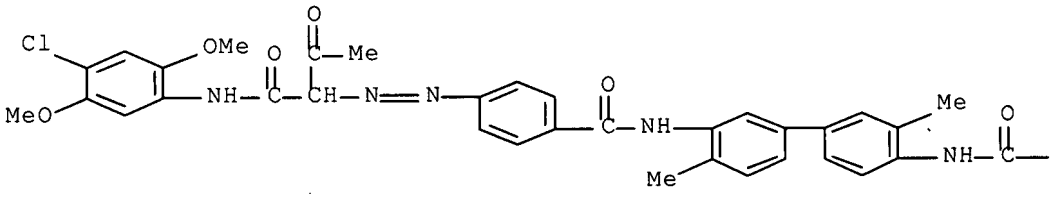
RN 873404-25-2 CAPLUS

CN 4',4'''-Bi-o-benzotoluidide, 4,4''-bis(-2-hydroxy-1-naphthylazo)- (5CI) (CA INDEX NAME)

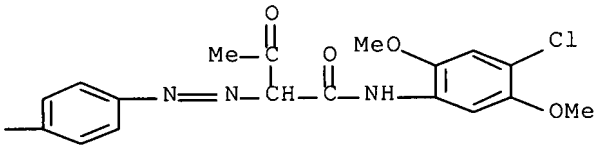


RN 873404-26-3 CAPLUS
CN 4',4'''-Bi-o-benzotoluidide, 4,4''-bis[1-[(4-chloro-2,5-dimethoxyphenyl)carbamoyl]acetonylazo]- (5CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L5 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1956:8382 CAPLUS Full-text
DN 50:8382
OREF 50:1687f-i,1688a-i,1689a-i,1690a-g
TI Anomalous Ullmann reactions. The unsymmetrical coupling of 2,6-dibromo-4-nitroiodobenzene
AU Carlin, Robert B.; Swakon, Edward A.
CS Carnegie Inst. of Technol., Pittsburgh, PA
SO Journal of the American Chemical Society (1955), 77, 966-73
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB When 2,6,4-Br2(O2N)C6H2I (I) was treated with Cu at 180-220°, the normal product, [2,6,4-Br2(O2N) C6H2] 2 (II), and the by-products,2,3',6- tribromo-2'-iodo-4,5'-dinitrobiphenyl (III), 2,6-bis(2,6-dibromo-4- nitrophenyl)-4-nitroiodobenzene (IV), and 3,5-Br2C6H3NO2 (V), were formed. The formation of III must be the result of an unsym. Ullmann coupling of I in which 1 of the 2 coupling mols. of I undergoes displacement of a Br atom rather than of the normally more active iodine atom, which in this case is further activated by a

NO2 group. The interaction of I and III undoubtedly accounts for the formation of IV. Powdered NaNO2 (25 g.) added slowly with vigorous stirring to 150 cc. concentrated H2SO4 at 0°, the mixture warmed to 70° until the solid dissolved, cooled to 15°, added at 15-25° gradually with stirring to a suspension of 75 g. 2,6-Br2C6H3NH2 in 600 cc. glacial AcOH, stirred to solution, diluted with 2 l. ice water, treated with 25 g. urea and then dropwise with 60 g. NaI in 300 cc. H2O, warmed to room temperature overnight, and treated with a little NaHSO3, and the buff-colored product recrystd. twice from Cellosolve gave 185-95 g. I, light tan needles, m. 153-5°. I (100 g.), 65 g. Cu, and 150 g. clean sand heated with stirring with a large paddle at 180°. the mixture kept 0.5 hr. at 210°, the resulting gray sludge boiled with four 500-cc. portions C6H6, the C6H6 extract passed through activated Al2O3, the light yellow effluent evaporated, the residue treated with 100 cc. Me2CO, the mixture refrigerated several hrs., and the solid deposit filtered off gave a mixture of II, III, and IV; the Me2CO filtrate containing some I, II, III, and V sublimed at 0.1 gave a mixture of I and V below 140° (the V was separated from the I by stream distillation); the fraction subliming at 140-90° was II, and that subliming at 190-235° was III; the dark, viscous, Me2CO-soluble residue congealed to a glass on cooling. A series of 5 Ullmann reactions with 100 g. I each carried out, the C6H6 exts. from the crude products of the 5 runs combined and the components separated in the usual manner gave in the Me2CO-insol. fraction 44 g. II, 54 g. III, and 16 IV; and in the Me2CO-soluble fraction 42 g. I, 60 g. II, 20 g. III, 18 g. V, and 55 g. resin. The crude II, light yellow flat needles, m. 174-5° (from MeOH) sublimed at 175° and 10-1 mm. gave pure II, cream-colored solid, m. 184.5-5.5°. The III, pale yellow needles, m. 233-3.5° (from C6H6), gave a pos. Na fusion test for iodine. The crude IV recrystd. from boiling PhCl once with and twice without C gave pure IV, yellow crystals, m. 388.5-90°. The crude V rapidly steam distilled and recrystd. 3 times from MeOH gave yellow crystals, m. 103-5.5°. II(2g.)and 0.7g. NaOH in 150cc. EtOH hydrogenated at room temperature over Raney Ni, the mixture filtered, concentrated, and poured into H2O, and the crystalline precipitate recrystd. from H2O gave 0.6 g. (p-H2NC6H4)2, m. 124-6.5°, which boiled 15 min. with Ac2O gave the N,N'-di-Ac derivative, white needles, m. 327-30° (from aqueous AcOH). Fe filings (100 g.) treated slowly with stirring with 20 cc. concentrated HCl and then dried over NaOH and KOH in vacuo gave activated Fe. Small amts. of H2O added periodically during 24 hrs. with stirring to 2.5 g. II and 100 g. activated Fe in 200 cc. boiling thiophene-free C6H6, the mixture filtered, the residue extracted with boiling C6H6, and half of the combined filtrate and washings concentrated to 20 cc., diluted with 20 cc. boiling cyclohexane, and cooled deposited 0.9 g. [4,2,6-H2N(Br2)C6H2]2 (VI), m. 249-50°; the filtrate gave an addnl. 0.1 g. VI. The other half of the solution of crude VI treated with a stream of ketene gave the N,N'-di-Ac derivative of VI, m. 336.5-8.5° (from aqueous AcOH). III reduced similarly with activated Fe and H2O, the filtered C6H6 solution subjected to the reduction once more the filtrate dried and distilled until the distillate was no longer cloudy, the dry solution cooled and treated with dry HCl, the precipitated HCl salt centrifuged off and dissolved in dilute HCl, the solution treated with concentrated aqueous NaOH, and the precipitate recrystd. 3 times from MeOH-cyclohexane, MeOH-C6H6, or C6H6-cyclohexane yielded 50% 4,5'-di-NH2 analog (VII) of III, colorless crystals, m. 250° (decomposition). Raney Ni (1 spoonful) (stored under EtOH) treated with 100 cc. C6H6, the mixture distilled until all EtOH was removed, the catalyst added to 7 g. III in 175 cc. dry C6H6 and a few cc. pyridine, the mixture hydrogenated 4 hrs. at room temperature and 3 atmospheric pressure, filtered, and treated with dry HCl, the precipitated viscous colorless oil centrifuged off, the solvent decanted, the residue dissolved in dilute HCl, the solution treated with concentrated NH4OH, and the precipitate recrystd. gave VII, light orange crystals, m. about 250° (decomposition) or 270° (decomposition), when inserted at 270°. N,N'-Di-Ac derivative (VIII) of VII (3.4 g.) in 30 cc. EtOH treated portionwise with 3 g. KOH in 6 cc. H2O, the

solution boiled 2 hrs., diluted with 30 cc. H2O, concentrated to 30 cc., poured into 50 cc. H2O, and refrigerated several hrs., and the crude product (2.9 g.) recrystd. from EtOH gave pure VII, white crystals, m. about 250° (decomposition). VII treated with BzCl in pyridine and C6H6 gave 30% N,N'-di-Bz derivative of VII, white needles, m. 185° (decomposition) (from MeOH-C6H6). Crude VII in C6H6 treated with ketene yielded 80-95% VIII. Boiling crude VII treated with a large excess of Ac2O containing a drop H2SO4 and the mixture poured into H2O precipitated 92-6% VIII; the crude VIII recrystd. from MeOH or sublimed at 250° and 10-4 mm. gave pure VIII, white crystals, m. 160-80°, resolidified at 180-205° and melted again at 280-3°. VIII recrystd. from aqueous AcOH gave cream-colored needles, m. 283-4°; VIII exists apparently in dimorphic modifications, the lower-melting form passing very readily into the higher-melting, more stable form. Crude VII, obtained by the Fe reduction of III, dissolved in 100 cc. concentrated HCl, the solution treated at 0° with stirring portionwise with 3 g. finely powdered NaNO2, the clear solution dropped into 500 cc. boiling EtOH, the solution filtered, concentrated to 75 cc., and cooled, and the resulting yellow-brown product (2.4 g.) sublimed at 140° and 0.010 mm. and recrystd. repeatedly from EtOH yielded 2,3',6-tribromo-2'-iodobiphenyl (IX), white needles, m. 156.5-58°. IX (0.9 g.) in 100 cc. EtOH hydrogenated 4 hrs. at room temperature and 3 atmospheric pressure over Raney Ni, the solution filtered, concentrated to 15 cc., poured into 300 cc. H2O, and refrigerated 4 hrs., and the solid deposit (0.2 g.) filtered and sublimed gave Ph2, m. 69-70.5°. VIII (5.75 g.) and 1.5 g. NaOH in 125 cc. EtOH hydrogenated 12 hrs. at room temperature and 3 atmospheric over 3 g. Raney Ni gave in the usual manner 1.8 g. 3,4'-diacetamidobiphenyl (X), white needles, m. 185-6.5°. X (2 g.) in 20 cc. boiling EtOH treated slowly with 4 cc. concentrated HCl, the solution cooled, the deposit (1.9 g.), m. 280° (decomposition), filtered, washed with absolute EtOH, and dissolved in 20 cc. H2O, the solution basified with aqueous NaOH and extracted with Et2O, the extract dried and evaporated, and the residue sublimed several times at 90° and 0.1 μ gave 0.65 g. 3,4'-diaminobiphenyl (XI), white crystalline solid, m. 85.5-6.5. BzCl (2 cc.) added dropwise into 0.55 g. XI in 15 cc. C6H6 and 6 cc. pyridine, the mixture warmed 1 hr. on the steam bath, poured into 100 cc. H2O, and filtered, and the filter residue (1.1 g.) washed and recrystd. from absolute EtOH gave the N,N'-di-Bz derivative, white needles, m. 223-4°. XI was converted by the method described previously (C.A. 45, 3341b) to the N,N'-bis(salicylal) derivative, yellow needles, m. 148-9° (from C6H6-heptane). p-AcNHC6H4Ph (XII) (35 g.) added with stirring to 400 cc. fuming HNO3 below 5°, the mixture stirred 0.5 hr., poured into H2O, and filtered, and the yellow solid washed and recrystd. from AcOH and then from Methyl Cellosolve gave 36 g. 3,4'-dinitro-4-acetamidobiphenyl (XIII), yellow crystals, m. 244-4.5°; method A. XII (50 g.) in 50 cc. glacial AcOH and 90 cc. concentrated H2SO4 treated slowly at 0° with 40 cc. HNO3 in 90 cc. glacial AcOH, the mixture warmed after 2 hrs. to room temperature, allowed to stand 24 hrs., and poured into 2 l. crushed ice, and the yellow precipitate filtered off, washed, and purified as in method A yielded 13 g. XIII, m. 241°. XIII (36 g.) in 120 cc. cold H2SO4 heated 2 hrs. on the steam bath, the dark solution poured onto 3 l. crushed ice, neutralized with NH4OH, and filtered, and the filter residue washed with H2O and recrystd. from Cellosolve gave 16 g. 3,4'-dinitro-4-aminobiphenyl (XIV), orange crystals, m. 230.5-2.5°. XIV deaminated in the usual manner yielded 78% 3,4'-dinitrobiphenyl (XV). long yellow needles, m. 186-8.5°. m-O2NC6H4Ph (XVI) (5 g.) stirred below 0° into 100 cc. fuming HNO3, the mixture poured onto crushed ice and filtered, the filter residue washed, dried, and digested with 170 cc. boiling MeOH, and the insol. material filtered off after cooling and sublimed at 155° and 0.001 mm. gave 2.1 g. XV, m. 185-8° (from C6H6-MeOH). m-O2NC6H4NH2 treated with 1.25 l. (instead of 3 l. C6H6) by the method of Bachmann and Hoffmann (C.A. 38, 2925.5), the excess PhNO2 steam distilled off, the residue dissolved in 1750 cc. C6H6, the solution passed through a column Al2O3, the C6H6 distilled off, the residue treated with 40 cc. Me2CO and refrigerated, and the resulting orange,

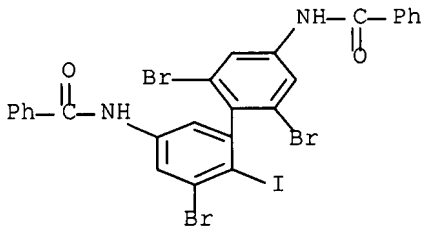
amorphous solid sublimed at 190° and 0.01 mm. yielded 11 g. XV, m. 187-8° (from C6H6-MeOH). XV (3 different samples, prepared by the 3 routes described) hydrogenated at room temperature and 3 atmospheric pressure over Raney Ni in C6H6, and the solution filtered and treated with ketene gave in each case X. IV in C6H6 containing a little pyridine hydrogenated by the method described for the reduction of III to VII, the precipitated HCl salts treated with dilute HCl, and the solid centrifuged, washed with H2O, and treated with NH4OH gave 0.9 g. 2,6-bis(2,6-dibromo-4-aminophenyl)-4-aminoiodobenzene (XVII), light tan crystals, m. about 315° (decomposition) (from C6H6-EtOH). N,N',N''-Tri-Ac derivative (XVIII) of XVII (0.5 g.) in 15 cc. 95% EtOH treated with 5 cc. concentrated HCl, the solution boiled 3 hrs., the resulting HCl salt (0.3 g.)filtered off, suspended in EtOH, and treated with aqueous NaOH, and the precipitate washed with H2O and EtOH and recrystd. twice from EtOH-C6H6 yielded 0.1 g. XVII, m. about 315° (decomposition). XVII treated with Ac2O containing a drop concentrated H2SO4 yielded 75% XVIII, white needles, m. 341-4° (decomposition) (from aqueous AcOH). IV reduced with activated Fe and H2O and the resulting solution treated with ketene also gave XVIII, m. 340-1°. IV (3.5 g.) in 600 cc. C6H6 treated at room temperature with Raney Ni and H at 3 atmospheric pressure, the mixture filtered, the filtrate concentrated to 50 cc,. diluted with excess EtOH, and distilled to remove the C6H6, the residue diluted with 0.85 g. NaOH in 100 cc. EtOH, the resulting solution hydrogenated 12 hrs. at room temperature and 3 atmospheric over 1 g. Raney Ni and filtered, the catalyst extracted with 100 cc. boiling EtOH and then 100 cc. boiling C6H6, and the combined filtrate and 2 exts. concentrated to 20 cc. and poured into 200 cc. cold H2O gave 1.2 g. white solid, presumably 3,5-bis(4-aminophenyl)aniline (XIX). XIX diazotized and converted to the corresponding triiodo derivative, the resulting brown solid (2.6 g.) in EtOH-C6H6 containing 1.5 g. NaOH hydrogenated 3 hrs. at 78° and 1000 lb. pressure over 1.5 g. Raney Ni, and the mixture filtered and worked up in a conventional manner gave 0.22 g. crude m-terphenyl (XX), m. 71-6°, which sublimed several times at 95° and 0.1 μ and recrystd. from EtOH and then MeOH gave pure XX, white needles, m. 86.5-87°. XVI (11 g.) in EtOH hydrogenated at room temperature and 3 atmospheric over Raney Ni gave m-H2NC6H4Ph (XXI), which was converted in 71% yield to m-IC6H4Ph, b5 164°. Crude XXI, prepared from 22 g. XVI, in 50 g. pyridine treated at 0° with stirring dropwise with 15 cc. AcCl the mixture allowed to stand 0.5 hr., poured into 1 l. cold dilute HCl, and the solid (23.3 g.) washed with H2O gave the N-Ac derivative (XXII) of XXI, m. 141-3°. NOCl (13 g.) in 25 cc. Ac2O added dropwise with stirring to 12 g. XXII, 100 cc. glacial AcOH, 30 cc. Ac2O, 15 g. KOAc, and 0.75 g. P2O5 at 5°, the mixture stirred 0.5 hr., poured into ice water, and extracted with C6H6, the extract washed with H2O, stirred 24 hrs. with 30 g. Na2SO4 and 25 g. Na2CO3 at room temperature, and filtered, the C6H6 and excess Ac2O removed in vacuo, the residue distilled, and the distillate (4.5 g.), yellow oil, b2-4 186-90°, cooled and recrystd. from MeOH gave XX, long white needles, m. 86.5-7,5°. 3,5-(H2N)2C6H3NO2 (24 g.) treated with 124 g. Ac2O, the mixture boiled 0.5 hr. and poured into 1 l. cold H2O gave 35 g. N,N'-di-Ac derivative (XXIII), yellow crystals, m. 270° (decomposition). NOCl (15 g.) in 40 cc. cold Ac2O added slowly with stirring to 17 g. XXIII, 100 cc. Ac2O, 200 cc. AcOH, 12 g. KOAc, and 1 g. P2O5 at 5°, the mixture stirred 1 hr., poured into 1.5 l. ice water, and extracted with PhNO2, the extract washed with 1% aqueous KOH, stirred 18 hrs. with 75 g. Na2CO3, filtered, distilled up to 205° (vapor temperature) and then steam distilled, the aqueous residue separated from the tars and extracted 3 days in a Soxhlet apparatus with C6H6, the C6H6 extract replaced by fresh C6H6, the solution again extracted 3 days, the combined exts. passed through a column Al2O3, and the light yellow effluent concentrated to 50 cc. and cooled deposited 5 g. solid mixture of at least 2 compds., m. 175° and about 270°, resp. The mixture (0.75 g.) chromatographed from 1 l. CCl4 on Al2O3, the chromatogram developed with C6H6 containing 0.2% EtOH, and the resulting yellow crystalline solid recrystd. from heptaneC6H6 yielded white crystals, m. 177-83°, possibly a trinitroterphenyl. The crude

mixed solid recrystd. from C6H6 and AcOH gave a small amount of insol. fraction; about 0.4 g. of this material dissolved in 120 cc. boiling C6H6, the solution filtered hot and cooled, the gelatinous deposit filtered off, dried, and recrystd. several times from Cellosolve gave about 0.1 g. of a trinitroterphenyl, yellow crystals, m. 263-8°, probably 3,5-(4-O2NC6H4)2C6H3NO2 (XXIV). XXIV (about 50 mg.) in 1:1 C6H6-EtOH hydrogenated at room temperature and 3 atmospheric pressure 4 hrs. over Raney Ni, the solvent removed on the steam bath, the residue dissolved in C6H6, the solution treated with ketene, and the product recrystd. from C6H6-EtOH gave 3,5-bis(4-acetamidophenyl)acetanilide (XXV), light tan needles, m. 311.5-13° (decomposition). XVIII (1.3 g.) and 1 g. NaOH in 150 cc. EtOH treated 12 hrs. with H at room temperature and 3 atmospheric over Raney Ni, the filtered solution concentrated to 25 cc. and poured into 50 cc. H2O, the solid precipitate filtered off, the crude filter residue (0.6 g.) dissolved in 200 cc. C6H6, the solution treated with ketene, concentrated to 30 cc., and cooled, and the resulting white solid deposit recrystd. from MeOH-C6H6 and from aqueous AcOH gave XXV, tan needles, m. 315° (decomposition).

IT 854209-47-5P, 3',4'''-Bibenzanilide, 3''',5',5'''-tribromo-4'-iodo-
854209-49-7P, 3',4'''-Bibenzanilide
RL: PREP (Preparation)
(preparation of)

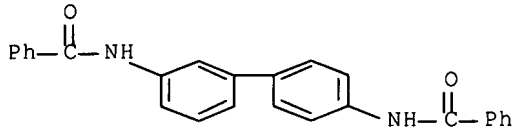
RN 854209-47-5 CAPLUS

CN 3',4'''-Bibenzanilide, 3''',5',5'''-tribromo-4'-iodo- (5CI) (CA INDEX NAME)



RN 854209-49-7 CAPLUS

CN 3',4'''-Bibenzanilide (5CI) (CA INDEX NAME)



L5 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1950:27412 CAPLUS Full-text

DN 44:27412

OREF 44:5363d-i,5364a-i,5365a

TI Potential trypanocides of the N-heterocyclic series. II. Analogs of dimidium bromide

AU Walls, L. P.; Whittaker, N.

CS Wellcome Research Labs., Beckenham, UK

SO Journal of the Chemical Society (1950) 41-7

CODEN: JCSOA9; ISSN: 0368-1769
DT Journal
LA Unavailable
OS CASREACT 44:27412

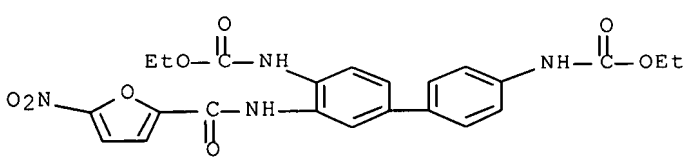
AB cf. C.A. 42, 4585a. The following phenanthridines were prepared for a study of the correlation of structure with trypanocidal activity. Cyclohexanecarbonyl chloride (26 g.), added to 52 g. 2,4-H2N(EtO2CNH)C6H3C6H4NHCO2Et-4 (I) in 75 mL. C5H5N and heated 15 min. on the steam bath, gives 63 g. 2-cyclohexylcarbonylamino-4, 4'-bis(carbethoxyamino)-biphenyl (II), m. 184-5°. II (63 g.) and 63 mL. POCl3, heated 45 min. at 130°, give 55 g. 3,8-bis(carbethoxyamino)-6-cyclohexylphenanthridine (III) (C.A. numbering), m. 233-4°; 2 g. III in 15 mL. PhNO2, treated 10 min. at 170° with 1.2 mL. Me2SO4, yielded the H sulfate, yellow, m. 227-8° (decomposition), but not a quaternary salt (probably because of steric hindrance). I (12 g.) in 130 mL. PhCl, treated with 5.5 g. PhCH2COCl and refluxed 30 min., gives 15.1 g. of the 2-phenylacetamido analog (IV) of II, m. 204-5°; 13.2 g. IV and 40 mL. POCl3, refluxed 1 h., give 11.4 g. of the 6-benzyl analog (V) of III, m. 259° (decomposition); 10 g. V in 80 mL. PhNO2 at 170°, treated with 10 mL. Me2SO4, heated 3 min. at 160-5°, and 2 N HCl added to the precipitate in H2O, gives 7.2 g. of the methochloride (VI), bright yellow, m. 254° (decomposition); 7.9 g. VI, 28 mL. concentrated H2SO4, and 24 mL. H2O, heated about 30 min. at 150°, give 5.8 g. 3,8-diamino-6-benzyl-5-methylphenanthridinium bromide, purple, m. 250-2°, highly trypanocidal (Trypanosoma congolense), although less effective than dimidium bromide (VII). I (70.5 g.) and 30 g. 2-thiophenecarbonyl chloride in 300 mL. PhNO2, heated 2 h. at 150° and left overnight, give 79 g. 2-(2-thenoylamino)-4,4'-bis(carbethoxyamino)biphenyl (VIII), m. 197-8°; 79 mg. VIII and 80 mL. POCl3, heated 75 min. at 130-5°, give 35 g. of the 6-(2-thienyl) analog of III, pale yellow, m. 229-30° (decomposition), purified through the HCl salt; the methochloride (IX), orange, m. 239° (decomposition); hydrolysis of 11.5 g. IX with H2SO4 at 135-40° gives 5.6 g. 3, 8-diamino-6-(2-thienyl)- 5-methylphenanthridinium bromide, deep purple, m. 256° (decomposition); this is a more effective trypanocide than VII. I (75 g.) and 39 g. 5-nitro-2-furoyl chloride in 150 mL. C5H5N give 95 g. of the 3-(5-nitro-2-furoylamino) analog (X) of II, yellow brown, m. 223-5°; 95 g. X yields 15.5 g. of the 6-(5-nitro-2-furyl) analog of III, with C5H5N of crystallization (lost at 125°), yellow-brown, m. 286-8° (decomposition); attempts to form quaternary salts caused profound decomposition I (27.5 g.) yields 27 g. of the 3-(3-pyridyl-carbonylamino) analog (XI) of II, m. 228-9° (decomposition) [methiodide, m. 162° (decomposition)]. XI (46 g.), 46 mL. POCl3, and 46 mL. PhNO2, heated 1 h. at 130°, give 9 g. of the 6-(3-pyridyl) analog (XII) of III, m. 196-8° (decomposition). XII (10.6 g.), 11 mL. MeI, and 50 mL. dioxane, refluxed 1 h. and the resulting gum in 250 mL. hot H2O containing a little AcOH treated with 2-C10H7SO3H, give 9.9 g. of the 1'-(metho-2-naphthalenesulfonate) 5-(2-naphthalenesulfonate), m. 228-9° (decomposition); boiled with aqueous AcONa it yields the 1'-(metho-2-naphthalenesulfonate), yellow, m. 142° (decomposition); this is probably the pyridinium salt and not the phenanthridinium salt. Attempts to hydrolyze the urethane groups did not lead to crystalline products. I (24 g.) yields 21.5 g. of the 3-(5,6-dihydro-3-pyranylcarbonylamino) analog of II, m. 186-8°; this affords 15% of the 6-(5,6-dihydro-3-pyranyl) analog of III, m. 215-16° [(methochloride, yellow, m. 260° (decomposition)]; this could not be hydrolyzed without attack of the dihydropyran ring. I (69 g.) and 42 g. 4-O2N-C6H4COCl in 280 mL. PhNO2, heated 30 min. at 150°, give 84 g. 2-(p-nitrobenzamido)-4,4'-bis(carbethoxyamino)-biphenyl (XIII), yellow, m. 202°; 80 g. XIII with POCl3 gives 46 g. 3,8-bis(carbethoxyamino)-6- (p-nitrophenyl)-phenanthridine (XIV), yellow, m. about 247° (decomposition). XIV (82 g.) and 70 mL. Me2SO4 in 500 mL. PhNO2 give 96 g. 3,8-bis(carbethoxyamino)-6-(p-nitrophenyl)-5-methylphenanthridinium Me sulfate, orange, m. about 240-1° (decomposition); hydrolysis with H2SO4 (d. 1.66) (30 min. at 125-30°) gives 51.5 g. 3, 8-

diamino-6-(p-nitrophenyl)-5-methylphenanthridinium chloride (XV), dark purple, m. about 235° (decomposition). XV (5 g.) in 50 mL. AcOH, heated 30 min. on the steam bath with 10 mL. Ac2O, gives 4.7 g. of the di-Ac derivative (XVI), orange, m. above 300°. Reduction of XVI with Fe and H2O was unsatisfactory; however, a 30% excess of Fe(OH)2 (30 min. on the water bath) gives a nearly quant. yield of the 6-(p-aminophenyl) analog (XVII) of XVI, yellow, m. about 280-1° (decomposition); 6.05 g. XVII and 60 mL. 2 N HCl, refluxed 1 h., give 4.7 g. 3,8-diamino-6-(p-aminophenyl)-5- methylphenanthridinium chloride (XVIII), dark red, m. about 240° (decomposition); reduction of 30.5 g. XV with Fe(OH)2 gives 26.2 g. XVIII. 2,4-H2N(O2N) C6H3-C6H4NO2-4 and 4-O2NC6H4COCl in boiling PhNO2 give a nearly quant. yield of 3-(p-nitrobenzamido)-1,4'-dinitrobiphenyl, yellow, m. 234°; with POCl3 in PhNO2 there results a nearly quant. yield of 3,8-dinitro-6-(p-nitrophenyl)phenanthridine (XIX), cream, m. 356-8°; it does not yield quaternary salts; 5 g. XIX in 125 mL. EtOH, treated with 25 mL. concentrated HCl and 30 g. SnCl22H2O and refluxed 2 h., gives 3, 8-diamino-6-(p-amino-phenyl)phenanthridine, yellow, m. 246°, devoid of trypanocidal activity; the tri-Ac derivative (cream, m. 312°) with Me2SO4 in PhNO2 at 180° gives a rather poor yield of 3,4', 8-triacetamido-6-phenyl-5-methylphenanthridinium sulfate, orange, m. 248° (decomposition); hydrolysis with 10% MeOH-HCl gives XVIII. Both XV and XVIII are highly trypanocidal, the former being at least equal to VII in T. congolense infections in mice and dogs and the latter markedly more active and somewhat less (acutely) toxic. XVIII is also highly active in T. rhodesiense infections in mice; in this respect it much exceeds any other phenanthridinium compound yet investigated, being as active as pentamidine although more toxic. 2-(p-Methoxybenzamido)-4,4'- bis(carbethoxyamino)biphenyl (m. about 100-5°) yields 3,8-bis (carbethoxyamino)-6-(p-methoxyphenyl) phenanthridine, m. 190-2° (decomposition); methosulfate, deep yellow, m. about 230° (decomposition); the hydrolysis product could not be obtained crystalline, probably because of simultaneous hydrolysis of the MeO group. 3,8-Diamino-6- phenylphenanthridine (10 g.) and 18 g. anhydrous Na2CO3, refluxed 8 h. in 100 mL. MeOH, 24 mL. H2O, and 30 mL. MeI, give 14 g. 6-phenylphenanthridine- 3,8-bis(trimethyl-ammonium iodide), m. 255° (decomposition); heated 30 min. at 180°, it yields 3, 8-bis(dimethylamino)-6-phenyl-5- methylphenanthridinium iodide, black, m. 260-2° (decomposition); the corresponding bromide is purple and possesses the high antibacterial activity in vitro characteristic of phenanthridinium salts, but both salts are practically inactive against trypanosomes. This suggests that H bonding, or some other reaction between drug and substrate not possible with a tertiary amine, is associated with the trypanocidal action of VII and its analogs.

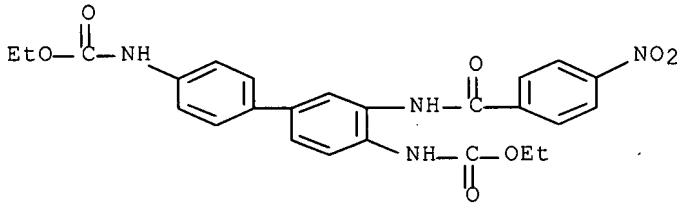
IT 854211-30-6P, 4,4'-Bicarbanilic acid, 2-(5-nitro-2-furamido)-, diethyl ester 854211-34-0P, 4,4'-Bicarbanilic acid, 2-p-nitrobenzamido-, diethyl ester 854211-53-3P, 4,4'-Bicarbanilic acid, 2-p-anisamido-, diethyl ester 858811-50-4P , 4,4'-Bicarbanilic acid, 2-nicotinamido-, diethyl ester 858811-53-7P, 4,4'-Bicarbanilic acid, 2-(2-thiophenecarboxamido)-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 854211-30-6 CAPLUS

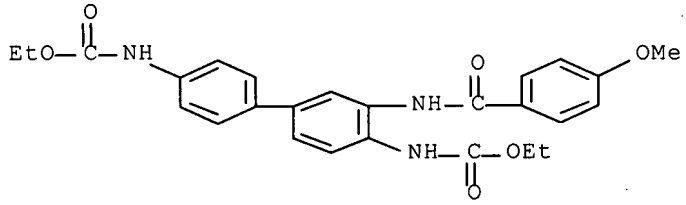
CN 4,4'-Bicarbanilic acid, 2-(5-nitro-2-furamido)-, diethyl ester (5CI) (CA INDEX NAME)



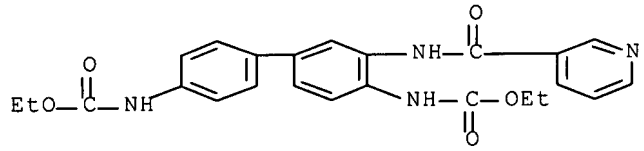
RN 854211-34-0 CAPLUS
CN 4,4'-Bicarbanilic acid, 2-p-nitrobenzamido-, diethyl ester (5CI) (CA INDEX NAME)



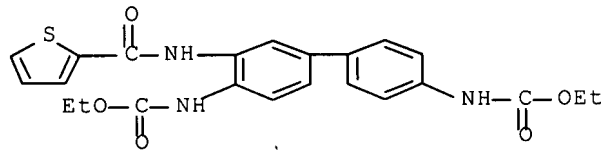
RN 854211-53-3 CAPLUS
CN 4,4'-Bicarbanilic acid, 2-p-anisamido-, diethyl ester (5CI) (CA INDEX NAME)



RN 858811-50-4 CAPLUS
CN 4,4'-Bicarbanilic acid, 2-nicotinamido-, diethyl ester (5CI) (CA INDEX NAME)



RN 858811-53-7 CAPLUS
CN 4,4'-Bicarbanilic acid, 2-(2-thiophenecarboxamido)-, diethyl ester (5CI) (CA INDEX NAME)



L5 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1948:2776 CAPLUS Full-text
DN 42:2776
OREF 42:622g-i,623a-c
TI Phenanthridine compounds
IN Walls, Leslie P.
DT Patent
LA Unavailable
FAN.CNT 1

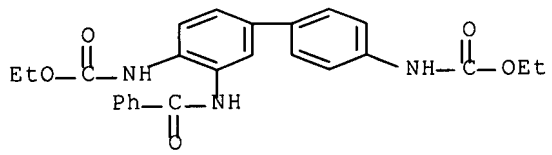
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 587673		19470502	GB	<--

GI For diagram(s), see printed CA Issue.

AB Quaternary salts of 3,8-diamino-6-phenylphenanthridine (I) of the general formula possess outstanding trypanocidal activity. I.MeBr is very powerfully active against Trypanosoma congolense infections in cattle, being generally curative in one dose, administered subcutaneously. It is also active to a lesser extent against T. brucei. Starting materials and procedures are similar to those already described (cf. Brit. 372,859, 511,353, and 578,226 in C.A. 27, 3483, 34, 6020.4, and 41, 2449g, resp., and U.S. 2,397,391 in C.A. 40, 4086.6). 2-Amino-4,4'-dinitrobiphenyl and BzCl gave a good yield of 2-benzamido-4,4'-dinitrobiphenyl (II), m. 234° (from HOAc or PhNO2). II with POCl3 in PhNO2 at 170-90° 20 hrs., followed by treatment with H2O, gave 45-55% 3,8-dinitro-6-phenylphenanthridine (III), m. 268°. III with Me2SO4 in PhNO2 at 190° 15 min., followed by steam distillation of the PhNO2, gave the 5-methosulfate of III, from which a pseudobase, m. 186-8°, was obtained by treatment with alkali. The 5-methochloride of III in aqueous solution was reduced with Fe, made alkaline with NH3, and filtered to remove a small amount of brownish impurity. The filtrate, upon addition of acid and KBr, precipitated I 5-methobromide, black or purple, m. 240° (decomposition). The 5-methochloride of I, purple-black, m. 250° (decomposition). Alternately, BzCl with 2-amino-4,4'-bis(carbethoxyamino)biphenyl gave the 2-benzamido derivative (IV), m. 147° (from AcOEt). Cyclization of IV by boiling 1 hr. with POCl3 gave 3,8-bis(carbethoxyamino)-6- phenylphenanthridine, which with Me2SO4 at 160° gave a theoretical yield of 3,8-bis(carbethoxyamino)-6-phenyl-5-methylphenanthridinium sulfate, yellow, m. 278° (decomposition). Hydrolysis with H2SO4 gave the 3,8-diamino quaternary salt.

IT 875853-91-1P, 4,4'-Bicarbanilic acid, 2-benzamido-, diethyl ester
RL: PREP (Preparation)
(preparation of)

RN 875853-91-1 CAPLUS
CN 4,4'-Bicarbanilic acid, 2-benzamido-, diethyl ester (5CI) (CA INDEX NAME)



L5 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1947:17194 CAPLUS Full-text
DN 41:17194
OREF 41:3465d-i,3466a-i,3467a
TI Phenanthridine series. VIII. Further investigation of trypanocidal types
AU Walls, Leslie P.; Browning, C. H.; Calver, K. M.; Leckie, M. W.

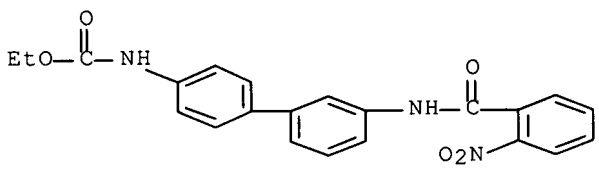
CS Dept. Sci. Ind. Research, Teddington, UK
SO Journal of the Chemical Society (1947) 67-74
CODEN: JCSOA9; ISSN: 0368-1769
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 41, 1682i. In Part VI (C.A. 39, 4326.4) it was shown that 9-phenylphenanthridinium salts with 2 NH2 groups exert a powerful chemotherapeutic action against T. congolense and it has been further demonstrated (C.A. 40, 3791.8) that similar salts with EtO2CNH in place of NH2 groups have some activity in T. crusi infections. In this paper the effect has been studied of replacing the 9-Ph by a 9-Me group and of substitution of I with other than NH2 groups; thus in different compds. R = NH2, NHAc, NHCO2Et, and R' or R'' = NO2, NH2, NHAc, or NHCO2Et. 2-(4-H2NC6H4)C6H4NHAc (10 g.) and 7.1 g. PhNEt2 in 50 mL. boiling EtOH, slowly treated with 3.5 mL. ClCO2Et, the mixture refluxed 30 min., and poured into 200 mL. N HCl, give 2-acetamido-4'-carbethoxyaminobiphenyl (II), m. 161°. II (6.5 g.) and 13 mL. POCl3, refluxed 1 h., give 5.2 g. 7-carbethoxyamino-9-methylphenanthridine (III), m. 210.5°. III and Me2SO4 in PhNO2 at 150° give 7-carbethoxyamino-9,10-dimethylphenanthridinium methosulfate, orange, characterized as the bromide, with 2 mols. H2O, deep yellow, m. 230° (decomposition). 7-Acetamido-9-methylphenanthridine yields a methosulfate, yellow, m. 270-2° (decomposition); hydrolysis with hot 5 N HCl, followed by neutralization and addition of KI, gives 7-amino-9,10- dimethylphenanthridinium iodide, brownish red, m. 261° (decomposition); chloride, brown, m. 260° (decomposition); bromide, orange-red, m. 269° (decomposition). 4-[2,4-O2N(EtO2CNH)C6H3]C6H4NHCO2Et, heated 1 h. with 20 mL. H2O, 1 drop HCl, and 5.5 g. reduced Fe, gives 2-amino-4,4'-bis(carbethoxyamino)biphenyl (IV), m. 186°; Ac derivative m. 199°. IV (36 g.) and 10.5 g. BzCl in 100 mL. PhNO2 at 150° give 35 g. of the Bz derivative, m. 147°; 20 g. and 40 mL. POCl3 refluxed 1 h., give 13.2 g. 2,7-dicarbethoxyamino-9- phenylphenanthridine, m. 222° (decomposition); methosulfate, orange, m. 278° (decomposition); H2SO4 gives a red acid sulfate, (C20H18N3)2SO 4.2.5H2SO4; KBr gives the purple bromide (C.A. 39, 4326.5). The Ac derivative of IV (5 g.) and 10 mL. POCl3 give 3.7 g. 2,7-bis(carbethoxyamino)-9- methylphenanthridine (V), m. 253° (decomposition); hydrolysis with H2SO4 gives 2,7-diamino-9-methylphenan-thridine, yellow, m. 265.5°; Ac derivative m. 323-6° (decomposition). V and Me2SO4 in PhNO2 at 160° give 2,7-bis(carbethoxyamino)-9,10-dimethylphenanthridinium methosulfate, yellow, does not m. up to 320°; chloride, yellow, does not m. up to 320°. 2,7-Diacetamido-9,10-dimethylphenanthridinium chloride, orange, does not m. up to 320°. Hydrolysis of either salt and addition of KBr give 2,7-diamino-9,10-dimethylphenanthridinium bromide, m. 283°; chloride, purple, m. 278°; iodide, dark purple, m. 293°. 2-O2NC6H4 C6H4NH2-4 (preparation given) (7 g.) gives 7 g. 2-nitro-4'-carbethoxyaminobiphenyl, yellow, m. 105.5°; reduction gives the 2-NH2 derivative (VI), m. 98°. VI (27 g.) and 23 g. p-O2NC6H4COCl in 88 mL. hot C5H5N give 36 g. 2-p-nitrobenzamido-4'- carbethoxyaminobiphenyl (VII), yellow, m. 184°. VII (21.5 g.), 72 mL. PhNO2, and 43 mL. POCl3, heated 1 h. at 150-60°, give 12.8 g. 7-carbethoxyamino-9-(p-nitrophenyl)phenanthridine (VIII), yellow, m. 254°; Me2SO4 in PhNO2 gives 7-carbethoxyamino-9-(p-nitrophenyl)-10- methylphenanthridinium methosulfate, orange, with 1 mol. H2O, m. 209° (decomposition); chloride, yellow, m. 243° (decomposition). Hydrolysis of VIII with H2SO4 gives 7-amino-9-(p- nitrophenyl)phenanthridine, red, m. 279°; Ac derivative, lemon-yellow, m. 282°; Me2SO4 gives a quant. yield of 7-acetamido-9-(p- nitrophenyl)-10-methylphenanthridinium methosulfate (IX), yellow, m. 267.5° (decomposition). Reduction of IX in hot H2O with Fe powder gives 7-acetamido-9-(p-aminophenyl)-10-methylphenanthridinium methosulfate, orange-yellow, m. 258° (decomposition); its aqueous solution with ClCO2Et gives 7-acetamido-9-(p-carbethoxyaminophenyl)-10-methylphenanthridinium chloride, with 3.5 mols. H2O, golden yellow, m. 200-6° (decomposition). 7-Carbethoxyamino-9-(p-aminophenyl)-10-methylphenanthridinium chloride m. 297-

300° (decomposition); Ac derivative m. 213° (decomposition). 7-Amino- 9-(p-nitrophenyl)-10-methylphenanthridinium chloride, dark red, m. 242° (decomposition). 4-Nitro-2'-o-nitrobenzamidobiphenyl, buff, m. 230-1°; POCl3 causes profound decomposition 4-EtO2CNHC6H4C6H4NH2-2 (10 g.) and 7.8 g. o-O2NC6H4COCl in 50 mL. boiling PhCl give 13.5 g. 2-o-nitrobenzamido-4'-carbethoxyaminobiphenyl, m. 197°; heating with POCl3 (1 h. on the steam bath) and purifying on Al2O3 give 7-carbethoxyamino-9-(o-nitrophenyl)phenanthridine, bright yellow, m. 199°; Me2SO4 in PhNO2 gives 7-carbethoxyamino-9-(o-nitrophenyl)-10- methylphenanthridinium methosulfate (X), with 2 mols. H2O, yellow, m. 226° (decomposition). 7-Amino-9-(o-nitrophenyl)phenanthridine, brown, m. 230°; Ac derivative m. 287.5°; 7-acetamido-9-(o-nitrophenyl)- 10-methylphenanthridinium methosulfate, with 1 mol. H2O, deep yellow, m. 283° (decomposition); reduction with SnCl2 and concentrated HCl in EtOH gives 7-acetamido-9-(o-aminophenyl)-10-methylphenanthridinium chloride, with 2 mols. H2O, deep yellow, m. 271.5° (decomposition). 7-Carbethoxyamino-9- (o-aminophenyl)-10-methylphenanthridinium chloride, with 1 mol. H2O, brown, m. 272° (decomposition); Ac derivative, with 2 mols. H2O, m. 203-5° (decomposition). Hydrolysis of X with H2SO4 gives 7-amino-9-(o-nitrophenyl)-10-methylphenanthridinium methosulfate, red oil; chloride m. 86°; reduction with Fe gives the 9-(o-aminophenyl) derivative, ruby-red, m. 158° (decomposition). 7-Acetamido-9-(o-acetamidophenyl)-10- methylphenanthridinium chloride, with 3 mols. H2O, buff, m. 240.5° (decomposition). Data are given for the therapeutic effect in mice infected with T. congolense (XI) and T. brucei (XII). XII is less susceptible than XI to phenanthridine compds. and a compound exhibiting a very high curative action against infections with XI may show little or no effect on XII in a dose 200 times as great; slight action on XII may be associated with relatively weak action on XI. Although a 9-Ph group is not essential for trypanocidal action, analogs with a 9-Me group are less active. When 1 primary NH2 group is present in the 7-position and another in the 9-Ph ring, it is practically immaterial whether the latter NH2 group occupies the o-, m-, or p-position, as far as concerns toxicity and action on XI. The corresponding Ac derivs. have low trypanocidal power. The presence of a NO2 instead of NH2 group in the Ph ring causes only a slight reduction in chemotherapeutic action. EtO2CNH and AcNH replacing the primary NH2 group in the phenanthridine ring reduce the therapeutic effect, while as a rule slightly decreasing toxicity. It appears that the presence of at least 1 NH2 group in the phenanthridine part is the most important factor for trypanocidal activity.

IT 848278-36-4P, Carbanilic acid, p-[m-[o-nitrobenzamido]phenyl]-, ethyl esters 848280-10-4P, Carbanilic acid, p-[m-[p-nitrobenzamido]phenyl]-, ethyl esters 875853-91-1P, 4,4'-Bicarbanilic acid, 2-benzamido-, diethyl ester
RL: PREP (Preparation)
(preparation of)

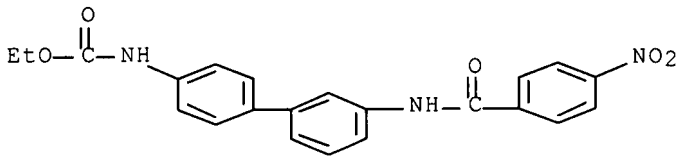
RN 848278-36-4 CAPLUS

CN Carbanilic acid, p-[m-[o-nitrobenzamido]phenyl]-, ethyl esters (5CI) (CA INDEX NAME)

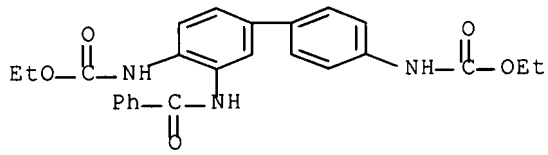


RN 848280-10-4 CAPLUS

CN Carbanilic acid, p-[m-[p-nitrobenzamido]phenyl]-, ethyl esters (5CI) (CA INDEX NAME)



RN 875853-91-1 CAPLUS
CN 4,4'-Bicarbanilic acid, 2-benzamido-, diethyl ester (5CI) (CA INDEX NAME)



=> s l4 not l5
L6 10 L4 NOT L5

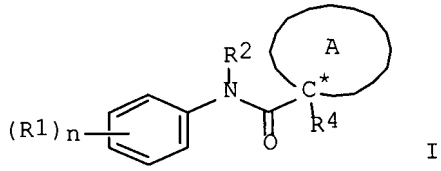
=> dis l6 1-10 bib abs fhitstr

L6 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:846121 CAPLUS Full-text
DN 147:211534
TI Cycloalkylcarboxamides and related compounds as modulators of ATP-binding cassette transporters and their preparation, pharmaceutical compositions and use in the treatment of diseases
IN Ruah, Sara S. Hadida; Miller, Mark T.; Bear, Brian; McCartney, Jason; Grootenhuis, Peter D. J.
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 249pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

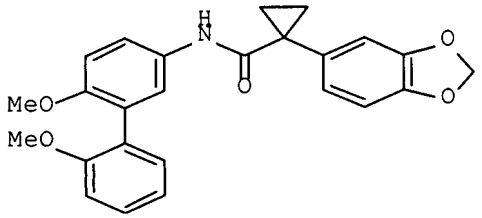
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007087066	A2	20070802	WO 2006-US49412	20061228

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

KG, KZ, MD, RU, TJ, TM
PRAI US 2005-754558P P 20051228
US 2006-802580P P 20060522
GI



I

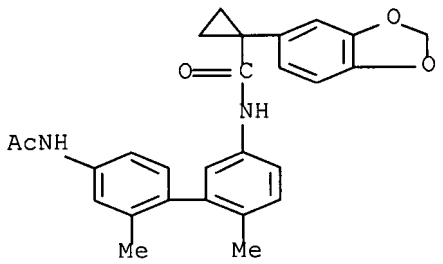


II

AB Compds. of formula I and pharmaceutically acceptable compns. thereof, are useful as modulators of ATP -Binding Cassette ("ABC") transporters or fragments thereof, including Cystic Fibrosis Transmembrane Conductance Regulator ("CFTR"). The invention also relates to methods of treating ABC transporter mediated diseases using compds. of formula I. Compds. of formula I wherein each R1 is independently (un)substituted C1-6 aliphatic, (un)substituted (hetero)aryl, (un)substituted C3-10 cycloaliph. and (un)substituted 4- to 10-membered heterocycloaliph., carboxy, amido, amino, halo and OH provided that at least one of R1 is (un)substituted (hetero)aryl attached to the 3- or 4-position of the Ph ring; R2 is H, (un)substituted C1-6 aliphatic, (un)substituted C3-6 cycloaliph., (un)substituted Ph, and (un)substituted heteroaryl; Ring A is (un)substituted cycloaliph., and (un)substituted heterocycloaliph. where the atoms of ring A adjacent to C* are carbon atoms; R4 is (un)substituted (hetero)aryl; n is 1, 2, 3, 4, and 5; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by a general procedure (procedure given). All the invention compds. were evaluated for their ATP-binding cassette transporter modulatory activity (some data given).

IT 945233-46-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of cycloalkylcarboxamides and related compds. as modulators of ATP-binding cassette transporters)

RN 945233-46-5 CAPLUS
CN Cyclopropanecarboxamide, N-[4'-(acetylamino)-2',6-dimethyl[1,1'-biphenyl]-3-yl]-1-(1,3-benzodioxol-5-yl)- (CA INDEX NAME)



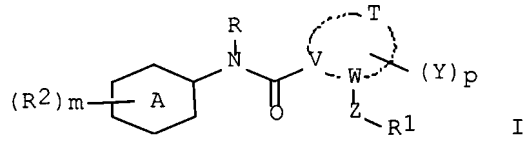
L6 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:670446 CAPLUS Full-text
DN 147:95910
TI Preparation of proline amides for treating Flaviviridae family virus infection
IN Schmitz, Franz Ulrich; Roberts, Christopher Don; Abadi, Ali Dehghani Mohammad; Griffith, Ronald Conrad; Leivers, Martin Robert
PA Genelabs Technologies, Inc., USA
SO PCT Int. Appl., 115pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007070556	A2	20070621	WO 2006-US47503	20061212
WO 2007070556	A3	20070830		

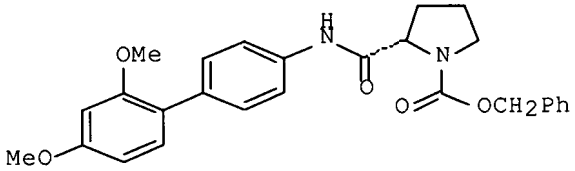
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRAI US 2005-749771P P 20051212
OS MARPAT 147:95910
GI



I



II

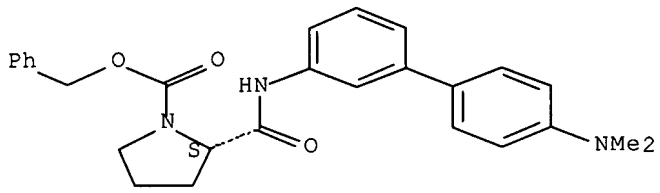
AB Title compds. I [wherein A = (un)substituted and optionally fused (N-hetero)aryl; R2 independently = (un)substituted alkyl, alkoxy, aryl, etc.; m = 1-3; R = H, (un)substituted alkyl or cycloalkyl; T is (hetero)alkylene and forms a ring with V and W; V and W are CH and N, at least of them being CH; Y = halo, oxo, OH or alkoxy; p = 0-2; Z = C(O), C(S) or SO2; R1 = (un)substituted amino, alkyl, alkoxy, etc., with limitations] and stereoisomers, tautomers, or pharmaceutically acceptable salts thereof, which are useful for treating or preventing a viral infection mediated at least in part by a virus in the Flaviviridae family of viruses, were prepared For instance, coupling of (S)-2-[(4- iodophenyl)carbamoyl]pyrrolidine-1-carboxylic acid benzyl ester with 2,4-dimethoxyphenylboronic acid gave proline amide II. This product showed 87.85% inhibition of hepatitis C virus (HCV) RNA dependent RNA polymerase at a concentration of 10 μM.

IT 942291-03-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of proline amides for treating Flaviviridae family virus infection)

RN 942291-03-4 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[4'-(dimethylamino)[1,1'-biphenyl]-3-yl]amino]carbonyl]-, phenylmethyl ester, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2007:538853 CAPLUS Full-text

DN 146:521690

TI Preparation of N-pyridinyl carboxamide derivatives as modulators of ATP-binding cassette transporters

IN Hadida Ruah, Sara; Hamilton, Matthew; Miller, Mark; Grootenhuis, Peter D. J.; Bear, Brian; Mccarthy, Jason; Zhou, Jinglan

PA Vertex Pharmaceuticals Incorporated, USA

SO PCT Int. Appl., 205pp.

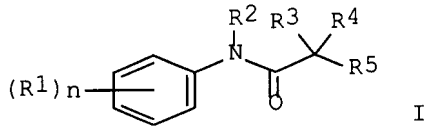
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007056341	A1	20070518	WO 2006-US43289	20061108

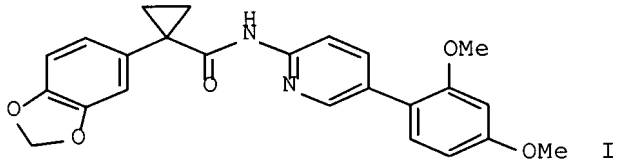
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI US 2005-734506P P 20051108
US 2005-754086P P 20051227
US 2006-802458P P 20060522
OS MARPAT 146:521690
GI



I

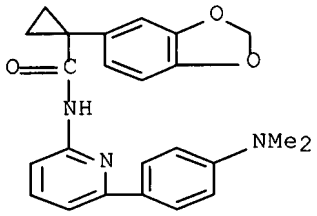


I

AB Title compds. I [R1 = (un)substituted alkyl, aryl, heteroaryl, etc.; R2 = H, (un)substituted alkyl, cycloalkyl, Ph, or heteroaryl; R3 and R4 together with the carbon to which they are attached form an (un)substituted cycloalkyl or heterocycloalkyl; R5 = (un)substituted aryl or heteroaryl; each n = 1-4], and pharmaceutically acceptable compns. thereof, are prepared and disclosed as useful as modulators of ATP-Binding Cassette ("ABC") transporters or fragments thereof, including Cystic Fibrosis Transmembrane Conductance Regulator ("CFTR"). Thus, e.g., the TFA salt of II was prepared by coupling of N-5-bromopyridin-2-yl 1-benzo[1,3]dioxol-5-ylcyclopropanecarboxamide (preparation given) with 2,4-dimethoxybenzeneboronic acid. I in bioassays described exhibited activity with a range of about 100 nM and 20 μM. The present invention also relates to methods of treating ABC transporter mediated diseases using compds. of the present invention.

IT 936722-18-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-pyridinyl carboxamide derivs. as modulators of atp-binding
cassette transporters)
RN 936722-18-8 CAPLUS
CN Cyclopropanecarboxamide, 1-(1,3-benzodioxol-5-yl)-N-[6-[4-(dimethylamino)phenyl]-2-pyridinyl]- (CA INDEX NAME)

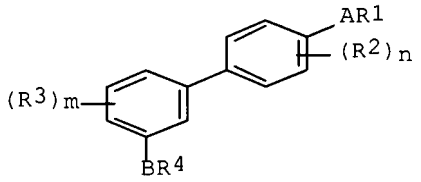


RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:327723 CAPLUS Full-text
DN 146:358864
TI Preparation of heterocyclyl biphenylcarboxamides for treatment of hepatitis C virus (HCV) infection.
IN Wheelhouse, Christopher James; Thomas, Alexander James Floyd; Bushnell, David John; Lumley, James; Salter, James Iain; Carter, Malcolm Clive; Mathews, Neil; Pilkington, Christopher John; Angell, Richard Martyn
PA Arrow Therapeutics Limited, UK
SO PCT Int. Appl., 170pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2007031791	A1	20070322	WO 2006-GB3469	20060918
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRAI GB 2005-18971	A	20050916		
GB 2006-10663	A	20060530		
GB 2006-10664	A	20060530		

OS MARPAT 146:358864
GI



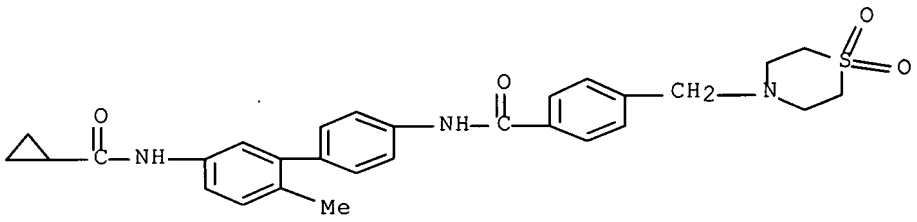
I

AB Title compds. [I; R1 = alkyl, A1, L1A1, A1A11, L1A1A11, A1L1A11, A1Y1A11, A1Het1A11, L1A1Y1A11, L1A1Het1A11, L1Het1A1, L1Y1A1, L1Y1Het1A1, L1Het1Y1A1, L1Y1Het1L11, A1Y1Het1A11, A1Het1Y1A11, A1Het1L1A11, A1L1Het1A11, L1Het1L11; A, B = bond, CONR', NR'CO, NR'CO2, CO, NR'CONR'', NR'SO2, SO2, NR', NR'COCO, CO2, alkylene-NR', hydroxyalkylene-NR'; R', R'' = H, alkyl; R2, R3 = alkyl, alkoxy, haloalkyl, haloalkoxy, halo; m, n = 0, 1; R4 = alkyl, A4, L4A4, A4A41, L4A4A41, A4L4A41, A4Y4A41, A4Het4A41, L4A4Y4A41, L4A4Het4A41, L4Het4A4, L4Y4A4, L4Y4Het4A4, L4Het4Y4A4, L4Y4Het4L41, A44Het4A41, A4Het4Y4A41, A4Het4L4A41, A4L4HetA41, L4Het4L41; A1, A4, A11, A41 = Ph, 5-10 membered heteroaryl, heterocyclyl, carbocyclyl; L1, L4 = alkylene, hydroxyalkylene; Y1, Y4 = CO, SO, SO2; L11, L41 = H, alkyl; Het1, Het4 = O, S, NR'; the Ph, heteroaryl, heterocyclyl and carbocyclyl moieties in R1, R4 being optionally substituted and/or fused to Ph, 5-10 membered heteroaryl, heterocyclyl], were prepared Thus, 6-methylbiphenyl-3,,4'-dicarboxylic acid 4'-[(4-isoxazol-5-ylphenyl)amide] 3-[(4-morpholin-4-ylphenyl)amide] (preparation outlined) inhibited HCV replication with IC50 <1 μM.

IT 929890-43-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyl biphenylcarboxamides for treatment of hepatitis
C virus infection)

RN 929890-43-7 CAPLUS

CN Benzamide, N-[5'-[(cyclopropylcarbonyl)amino]-2'-methyl[1,1'-biphenyl]-4-yl]-4-[(1,1-dioxido-4-thiomorpholinyl)methyl]- (CA INDEX NAME)



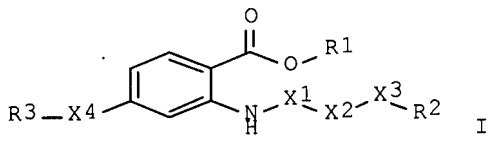
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:577803 CAPLUS Full-text
DN 145:62687
TI Preparation of N-acylanthranilic acid derivatives or salts thereof as inhibitor for production of matrix metalloproteinase (MMP-13)
IN Yokotani, Junichi; Taniguchi, Yoichi; Hara, Eiji; Akitsu, Hitoshi; Tada, Yukie
PA Toyama Chemical Co., Ltd., Japan

SO PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006062093	A1	20060615	WO 2005-JP22367	20051206
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005312721	A1	20060615	AU 2005-312721	20051206
CA 2588633	A1	20060615	CA 2005-2588633	20051206
EP 1820795	A1	20070822	EP 2005-814561	20051206
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
IN 2007KN01796	A	20070810	IN 2007-KN1796	20070521
PRAI JP 2004-353725	A	20041207		
WO 2005-JP22367	W	20051206		

OS MARPAT 145:62687
GI



I

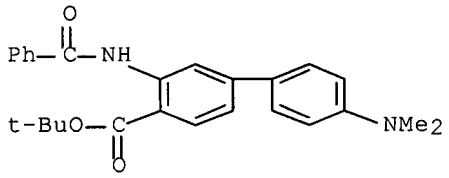
AB The title compds. [I; wherein R1 = H, a carboxy-protecting group; R2 = each (un)substituted Ph, cycloalkyl, or heterocyclic group; R3 = each (un)substituted Ph, cycloalkyl, cycloalkenyl, or monocyclic or bicyclic heterocyclic group; X1 = CO or SO2; X2 = a bond, each (un)substituted alkylene, alkenylene, or alkynylene; X3 = O, S, a bond; X4 = -X5-X6- or -X6-X5- (the left side bond is linked to R3) (wherein X5 = O, S, (un)protected NH, SO, SO2, a bond; X6 = each (un)substituted alkylene, alkenylene, or alkynylene)] or salts thereof are prepared These compds. have an MMP-13 production inhibitory activity and are hence useful as therapeutic agents for articular rheumatism, osteoarthritis, cancer, etc. Thus, Me 2-(benzoylamino)-4-bromobenzoate was coupled with benzofuran-2-boronic acid in the presence of polymer-supported Bis(acetato)bis(triphenylphosphine)palladium and Na2CO3 in N,N-dimethylacetamide at 90° for 11 h followed by saponification and acidification with 1.0 M aqueous HCl solution to give 2-(benzoylamino)-4-(3-methoxyphenyl)benzoic acid (II). II and 2-(benzoylamino)-4-((E)-2-(3-

chlorophenyl)vinyl)benzoic acid inhibited the IL-1β-stimulated production of MMP-13 in human cartilage-derived SW1353 cells by 95 and 99%, resp., at 30 μM.

IT 890316-33-3P, tert-Butyl 2-(benzoylamino)-4-[4-(dimethylamino)phenyl]benzoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of N-acylanthranilic acid derivs. as inhibitors for production of matrix metalloproteinase (MMP-13))

RN 890316-33-3 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3-(benzoylamino)-4'-(dimethylamino)-, 1,1-dimethylethyl ester (CA INDEX NAME)



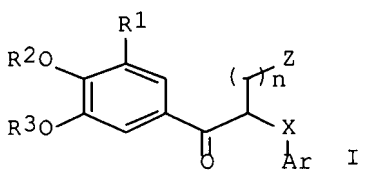
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:317273 CAPLUS Full-text
DN 144:369906
TI Preparation of benzamide derivatives as modulators of chemokine receptors for treatment of cancer
IN Melikian, Anita; Wright, John J. Kim
PA Chemocentryx, Inc., USA
SO U.S. Pat. Appl. Publ., 80 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

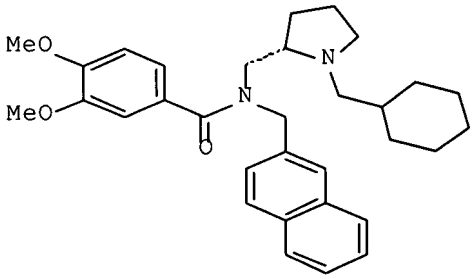
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2006074071	A1	20060406	US 2005-202961	20050811
WO 2006038989	A1	20060413	WO 2005-US29035	20050811

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI US 2004-614563P P 20040929
OS CASREACT 144:369906; MARPAT 144:369906
GI



I



II

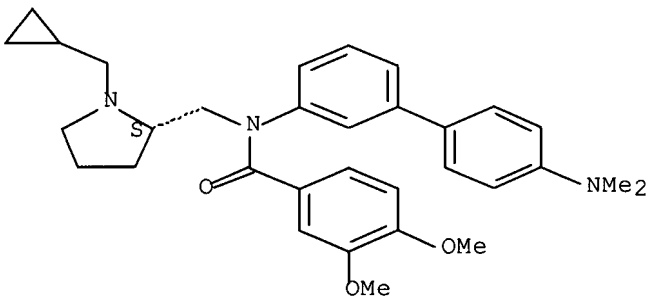
AB The title benzamide derivs. I [wherein n = 1-3; R1 = H, halo, (cyclo)alkyl, (cyclo)alkoxy, etc.; R2 and R3 = independently alkyl or haloalkyl; or R2 and R3 form a (un)substituted ring; X = a bond, CH2, or -CH(CH3)-; Ar = (un)substituted linked or fused bicyclic aromatic ring; Z = (un)substituted saturated nitrogen heterocyclic ring], or pharmaceutically acceptable salts thereof were prepared as modulators to inhibit the binding of the SDF-1 chemokine or I-TAC to the chemokine receptor CCXCKR2. For example, II was prepared in a multi-step synthesis. II showed inhibitory activity with IC50 ≤ 500 nM against the binding of SDF-1 to CCXCKR2 receptor. The compds. are useful for the treatment of cancer or inflammation (no data).

IT 882035-81-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzamide derivs. as modulators of CCXCKR2 for treatment of cancer)

RN 882035-81-6 CAPLUS

CN Benzamide, N-[[(2S)-1-(cyclopropylmethyl)-2-pyrrolidinyl]methyl]-N-[4'-(dimethylamino)[1,1'-biphenyl]-3-yl]-3,4-dimethoxy- (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:902755 CAPLUS Full-text

DN 143:242051

TI Compounds and compositions as LXR modulators

IN Molteni, Valentina; Li, Xiaolin; Liang, Fang; Nabakka, Juliet; Saez, Enrique; Wityak, John

PA IRM LLC, Bermuda

SO PCT Int. Appl., 51 pp.

CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005077122	A2	20050825	WO 2005-US4652	20050211
WO 2005077122	A3	20051229		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005211807	A1	20050825	AU 2005-211807	20050211
CA 2553442	A1	20050825	CA 2005-2553442	20050211
EP 1713465	A2	20061025	EP 2005-723051	20050211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1917870	A	20070221	CN 2005-80004674	20050211
BR 2005007626	A	20070703	BR 2005-7626	20050211
JP 2007523087	T	20070816	JP 2006-553323	20050211
IN 2006CN02907	A	20070608	IN 2006-CN2907	20060808
MX 2006PA09159	A	20061110	MX 2006-PA9159	20060811
PRAI US 2004-544149P	P	20040211		
WO 2005-US4652	W	20050211		

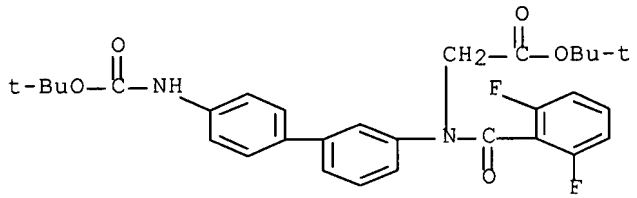
OS MARPAT 143:242051

AB The invention provides compds., pharmaceutical compns. comprising such compds. and methods of using such compds. to treat or prevent diseases or disorders associated with the activity of liver X receptors (LXRs).

IT 863093-34-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(compds. and compns. as liver X receptor modulators for treatment of diseases and combination with other agents)

RN 863093-34-9 CAPLUS

CN Glycine, N-(2,6-difluorobenzoyl)-N-[4'-[[(1,1-dimethylethoxy)carbonyl]amino][1,1'-biphenyl]-3-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

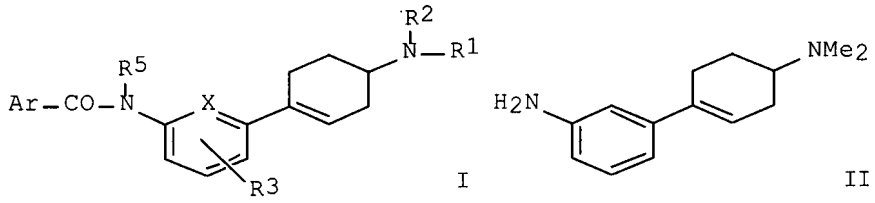


L6 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:588871 CAPLUS Full-text
DN 143:115447
TI Preparation of (4-aminocyclohexen-1-yl)pyridines and relate compounds as 5-HT1F agonists for the treatment of migraines
IN Kohlman, Daniel Timothy; Victor, Frantz; Xu, Yao-Chang; Ying, Bai-Ping; Zhang, Deyi
PA Eli Lilly and Company, USA
SO PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

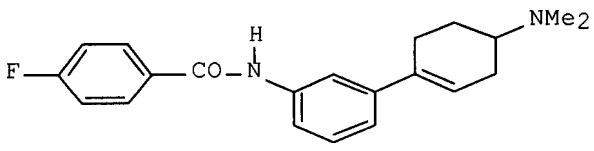
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005061439	A1	20050707	WO 2004-US38226	20041206
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2549007	A1	20050707	CA 2004-2549007	20041206
	EP 1697305	A1	20060906	EP 2004-816953	20041206
	EP 1697305	B1	20070815		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
	JP 2007516266	T	20070621	JP 2006-545653	20041206
	US 2007078169	A1	20070405	US 2006-576762	20060421
PRAI	US 2003-530463P	P	20031217		
	WO 2004-US38226	W	20041206		

OS CASREACT 143:115447; MARPAT 143:115447
GI



I

II



III

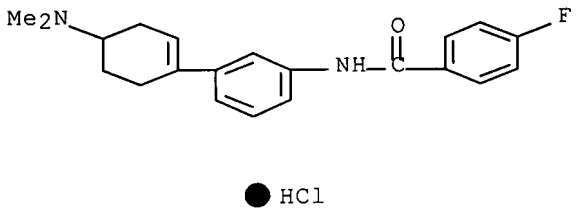
AB Title compds. I [X = C(R4), N; Ar = (un)substituted Ph, heterocycle; R1, R2 = H, alkyl; R3 = H, F, CH3; R4 = H, F, CH3 with provisos; R5 = H, CH3, CH2CH3]

and their pharmaceutically acceptable salts were prepared For example, N-benzoylation of aniline II with 4-fluorobenzoyl chloride afforded benzamide III in 74% yield. Compds. I were found to be agonist of the 5-HT1F receptor (no data provided).

IT 857335-08-1P, N-[3-(4-Dimethylaminocyclohex-1-enyl)phenyl]-4-fluorobenzamide hydrochloride salt
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminocyclohexenylpyridines and relate compds. as 5-HT1F agonists for the treatment of migraines)

RN 857335-08-1 CAPLUS

CN Benzamide, N-[3-[4-(dimethylamino)-1-cyclohexen-1-yl]phenyl]-4-fluoro-, monohydrochloride (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:300395 CAPLUS Full-text

DN 142:355054

TI Preparation of amide derivatives as inhibitors of histone deacetylase

IN Moradei, Oscar; Paquin, Isabelle; Leit, Silvana; Frechette, Sylvie; Vaisburg, Arkadii; Besterman, Jeffrey M.; Tessier, Pierre; Mallais, Tammy C.

PA Methylgene, Inc., Can.

SO PCT Int. Appl., 559 pp.
CODEN: PIXXD2

DT Patent

LA English

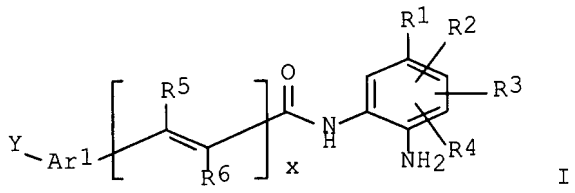
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005030705	A1	20050407	WO 2004-US31591	20040924
WO 2005030705	A9	20060420		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004276337	A1	20050407	AU 2004-276337	20040924
CA 2539117	A1	20050407	CA 2004-2539117	20040924

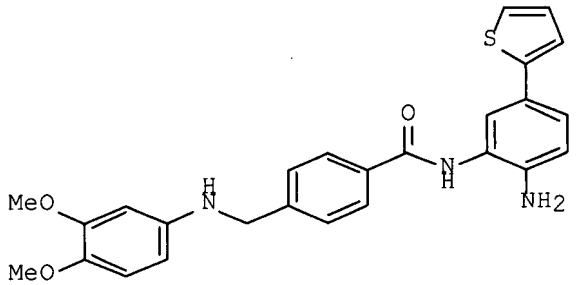
	EP 1663953	A1	20060607	EP 2004-789074	20040924
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
	CN 1882529	A	20061220	CN 2004-80034571	20040924
	JP 2007506785	T	20070322	JP 2006-528279	20040924
PRAI	US 2003-505884P	P	20030924		
	US 2003-532973P	P	20031229		
	US 2004-561082P	P	20040409		
	WO 2004-US31591	W	20040924		

OS MARPAT 142:355054

GI



I



II

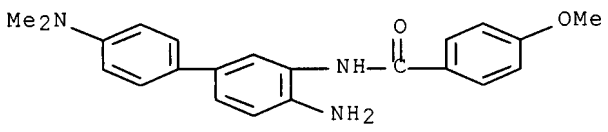
AB Title compds. I [Ar1 = (un)saturated-, (un)substituted-mono or fused polycyclic hydrocarbyl optionally containing 1-4 heteroatoms per ring; R1 = (un)substituted-mono-, -bi-, -tri-cyclic-aryl or -heteroaryl; R2, R3, and R4 independently = H, halo, amino, etc.; R5 and R6 independently = H, alkyl, aryl, etc.; x = 0-1; Y = any pharmaceutically acceptable chemical moiety consisting of 1 to 50 atoms with provisions] and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of histone deacetylase. Thus, e.g., II was prepared by Suzuki coupling of 2-bromo-2-nitro-phenylamine (preparation given) with 2-thiopheneboronic acid followed by carbonylation with 4-[3,4-dimethoxy-(phenylamino)- methyl]benzoic acid (preparation given) and subsequent reduction The inhibitory capability of I towards antiproliferative activity of histone deacetylase enzyme was evaluated using 3-[4,5-dimethylthiazol-2-yl-2,5- diphenyltetrazolium] bromide (MTT) assay and it revealed that certain compds. of the invention had MTT IC 50 values in the range of below 1 up to 20 μM. I as histone deacetylase inhibitors should prove useful in the treatment of diseases such as, but not limited to, cell proliferative disease, protozoal disease, and fungal disease.

IT 849233-36-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amide derivs. as inhibitors of histone deacetylase)

RN 849233-36-9 CAPLUS
CN Benzamide, N-[4-amino-4'-(dimethylamino)[1,1'-biphenyl]-3-yl]-4-methoxy- (9CI) (CA INDEX NAME)

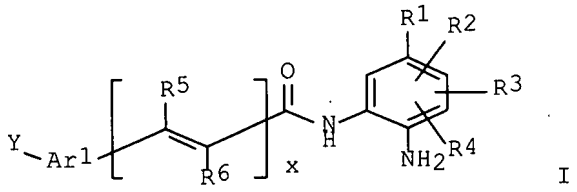


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

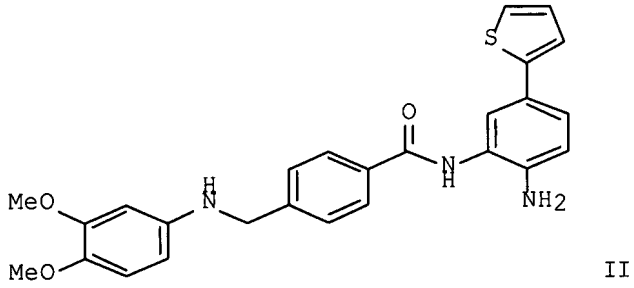
L6 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:300394 CAPLUS Full-text
DN 142:373563
TI Preparation of amide derivatives as inhibitors of histone deacetylase
IN Moradei, Oscar; Paquin, Isabelle; Leit, Silvana; Frechette, Sylvie; Vaisburg, Arkadii; Besterman, Jeffrey M.; Tessier, Pierre; Mallais, Tammy C.
PA Methylgene, Inc., Can.
SO PCT Int. Appl., 389 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005030704	A1	20050407	WO 2004-US31590	20040924
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2003-505884P	P	20030924		
	US 2003-532973P	P	20031229		
	US 2004-561082P	P	20040409		

OS MARPAT 142:373563
GI



I



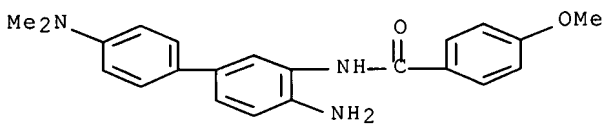
II

AB Title compds. I [Ar1 = (un)saturated-, (un)substituted-mono or fused polycyclic hydrocarbyl optionally containing 1-4 heteroatoms per ring; R1 = (un)substituted-mono-, -bi-, -tri-cyclic-aryl or -heteroaryl; R2, R3, and R4 independently = H, halo, amino, etc.; R5 and R6 independently = H, alkyl, aryl, etc.; x = 0-1; Y = any pharmaceutically acceptable chemical moiety consisting of 1 to 50 atoms with provisions] and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of histone deacetylase. Thus, e.g., II was prepared by Suzuki coupling of 2-bromo-2-nitro-phenylamine (preparation given) with 2-thiopheneboronic acid followed by carbonylation with 4-[3,4-dimethoxy-(phenylamino)- methyl]benzoic acid (preparation given) and subsequent reduction The inhibitory capability of I towards antiproliferative activity of histone deacetylase enzyme was evaluated using 3-[4,5-dimethylthiazol-2-yl-2,5- diphenyltetrazolium] bromide (MTT) assay and it revealed that certain compds. of the invention had MTT IC 50 values in the range of below 1 up to 20 μM. I as histone deacetylase inhibitors should prove useful in the treatment of diseases such as, but not limited to, cell proliferative disease, protozoal disease, and fungal disease.

IT 849233-36-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amide derivs. as inhibitors of histone deacetylase)

RN 849233-36-9 CAPLUS

CN Benzamide, N-[4-amino-4'-(dimethylamino)[1,1'-biphenyl]-3-yl]-4-methoxy- (9CI) (CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> log y
STN INTERNATIONAL LOGOFF AT 17:32:04 ON 20 SEP 2007
```